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FILE COVERS 1907 - 19 May 2004 VOL 140 ISS 21  
FILE LAST UPDATED: 18 May 2004 (20040518/ED)

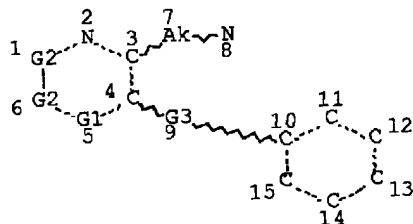
This file contains CAS Registry Numbers for easy and accurate substance identification.

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L19 STR



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VAR G2=C/N

VAR G3=S/C

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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

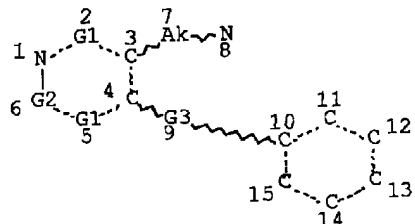
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NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

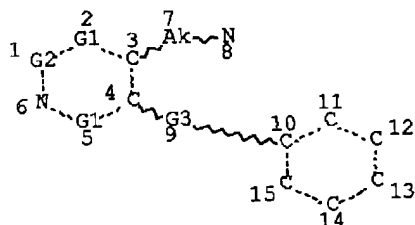
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DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 15

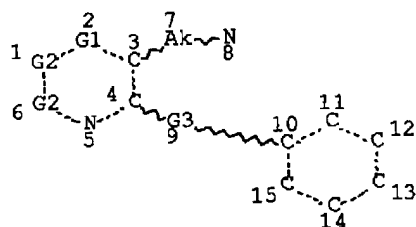
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L21 STR



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VAR G3=S/C  
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DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE  
L22 STR

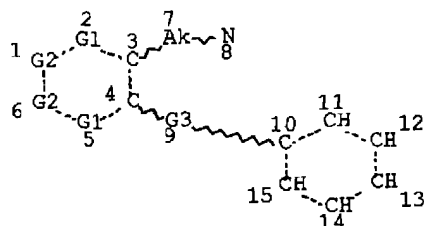


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NODE ATTRIBUTES:  
NSPEC IS RC AT 8  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

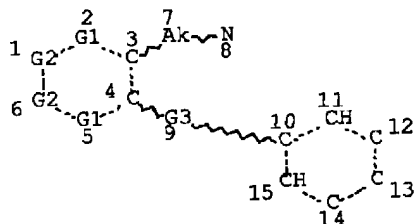
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L25 STR



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VAR G2=C/N  
VAR G3=S/CH2  
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NSPEC IS RC AT 8  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE  
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NOT L25  
L27 STR



VAR G1=CH/N  
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NODE ATTRIBUTES:  
NSPEC IS RC AT 8  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 15

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L29 71 SEA FILE=HCAPLUS ABB=ON PLU=ON L28  
L30 61 SEA FILE=HCAPLUS ABB=ON PLU=ON L29 AND PD=<AUGUST 16, 2002

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L30 ANSWER 1 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

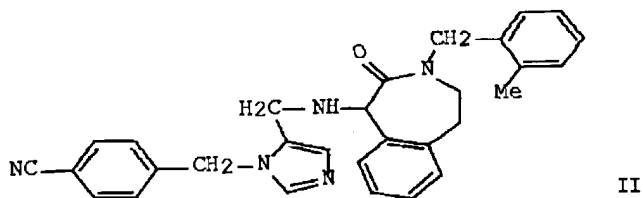
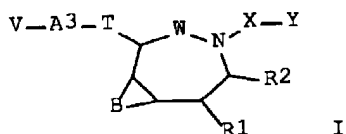
ACCESSION NUMBER: 2003:887694 HCAPLUS  
DOCUMENT NUMBER: 139:358745  
TITLE: Polyamine analogues as therapeutic and diagnostic agents  
INVENTOR(S): Vermeulin, Nicolaas M. J.; O'Day, Christine L.; Webb, Heather K.; Burns, Mark R.; Bergstrom, Donald E.  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S., 78 pp., Cont.-in-part of U.S. Ser. No. 396,523.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 4  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6646149	B1	20031111	US 2000-584175	20000531
WO 9903823	A2	19990128	WO 1998-US14896	19980715 <--
WO 9903823	A3	19990408		
W: AL, AM, AU, AZ, BA, BB, BG, BR, CA, CN, CU, CZ, EE, FI, GE, HU, IL, IS, JP, KG, KP, KR, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6172261	B1	20010109	US 1999-341400	19990903 <--
WO 2001092218	A2	20011206	WO 2001-US17795	20010531 <--
WO 2001092218	A3	20030327		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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EP 1317424	A2	20030611	EP 2001-946044	20010531
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004509845	T2	20040402	JP 2002-500833	20010531
PRIORITY APPLN. INFO.:				
US 1997-52586P P 19970715				
US 1997-65728P P 19971114				
US 1998-85538P P 19980515				
WO 1998-US14896 A2 19980715				
US 1999-341400 A2 19990903				
US 1999-396523 A2 19990915				
US 2000-584175 A 20000531				
WO 2001-US17795 W 20010531				
AB	Novel "bispolyamine" inhibitor compds. of polyamine transport are disclosed. These compds. are useful pharmaceutical agents for treating diseases where it is desired to inhibit polyamine transport or other polyamine binding proteins, for example cancer and post-angioplasty injury. These compds. display desirable activities both for diagnostic and research assays and therapy.			
IT	220221-36-3 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (novel polyamine transport-inhibiting polyamine analogs as therapeutic and diagnostic agents)			

L30 ANSWER 2 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:555486 HCAPLUS  
DOCUMENT NUMBER: 137:125099  
TITLE: Cyclo[d]azepane derivatives as farnesyl transferase inhibitors  
INVENTOR(S): Casara, Patrick; Le Diguarher, Thierry; Dorey, Gilbert; Hickman, John; Pierre, Alain; Tucker, Gordon; Guilbaud, Nicolas; Fauchere, Jean-Luc; Ortuno, Jean-Claude  
PATENT ASSIGNEE(S): Les Laboratoires Servier, Fr.  
SOURCE: PCT Int. Appl., 85 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: French  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057258	A1	20020725	WO 2002-FR149	20020116 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
FR 2819512	A1	20020719	FR 2001-639	20010118 <--
FR 2819512	B1	20030221		
PRIORITY APPLN. INFO.:			FR 2001-639	A 20010118
OTHER SOURCE(S):			MARPAT 137:125099	
GI				



AB Title compds. I [X = alkylene, CO, S(O)n, S(O)nA1, COA1, A1S(O)nA2, A1COA2; Y = (un)substituted aryl, heteroaryl, cycloalkyl, heterocycloalkyl; W = CO, CH2; R1, R2 = H, (un)substituted aryl, heteroaryl, cycloalkyl, heterocycloalkyl; T = CHR3, NR3, NR3CO; V = H, (un)substituted aryl, heteroaryl; A1, A2 = alkylene; A3 = (CR4R5)p; R3 = H, (un)substituted alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl; R4, R5 = H, (un)substituted alkyl, alkenyl, alkynyl, aryl, heteroaryl, heterocycloalkyl, aralkyl, heteroaralkyl, heterocyclylalkyl; B = atoms required to complete an (un)substituted aryl or heteroaryl ring; n = 0-2;

p = 0-4] were prepd. for use as farnesyl transferase inhibitors in the treatment of cancers, neurofibromatosis type 1 and restenosis after angioplasty or vascular surgery. Thus, 1-amino-3-(2-methylbenzyl)-1,3,4,5-tetrahydro-2H-3-benzazepin-2-one was prepd. from glyoxylic acid in 6 steps and was treated with 1-(4-cyanobenzyl)-1H-imidazole-5 carboxaldehyde to give the title compd. II.

IT 443927-03-5P 443927-04-6P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of cyclo[d]azepane derivs. as farnesyl transferase inhibitors)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 3 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:555485 HCAPLUS

DOCUMENT NUMBER: 137:125098

TITLE: Cyclo[c]azepane derivatives for use as farnesyltransferase inhibitors

INVENTOR(S): Casara, Patrick; Le Diguarher, Thierry; Dorey, Gilbert; Hickman, John; Pierre, Alain; Tucker, Gordon; Guilbaud, Nicolas; Fauchere, Jean-Luc; Ortuno, Jean-Claude

PATENT ASSIGNEE(S): Les Laboratoires Servier, Fr.

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

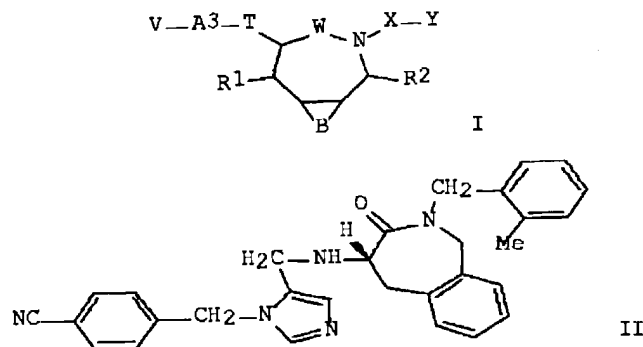
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057257	A1	20020725	WO 2002-FR148	20020116 <--
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RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
FR 2819510	A1	20020719	FR 2001-642	20010118 <--
FR 2819510	B1	20031031		

PRIORITY APPLN. INFO.: FR 2001-642 A 20010118

OTHER SOURCE(S): MARPAT 137:125098

GI



AB Title compds. I [X = alkylene, CO, S(O)n, S(O)nA1, COA1, A1S(O)nA2, A1COA2; Y = (un)substituted aryl, heteroaryl, cycloalkyl, heterocycloalkyl; W = CO, CH2; R1, R2 = H, (un)substituted aryl, heteroaryl, cycloalkyl, heterocycloalkyl; T = CHR3, NR3, NR3CO; V = H, (un)substituted aryl, heteroaryl; A1, A2 = alkylene; A3 = (CR4R5)p; R3 = H, (un)substituted alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl; R4, R5 = H, (un)substituted alkyl, alkenyl, alkynyl, aryl, heteroaryl, heterocycloalkyl, aralkyl, heteroaralkyl, heterocyclylalkyl; B = atoms required to complete an (un)substituted aryl or heteroaryl ring; n = 0-2; p = 0-4] were prepd. for use as farnesyl transferase inhibitors in the treatment of cancers, neurofibromatosis type 1 and restenosis after angioplasty or vascular surgery. Thus, (S)-4-amino-2-(2-methylbenzyl)-1,2,4,5-tetrahydro-3H-2-benzazepin-3-one was prepd. from H-L-Phe-NH2. HCl in 5 steps and was treated with 1-(4-cyanobenzyl)-1H-imidazole-5-carboxaldehyde to give the title compd. II.

IT **443926-06-5P 443926-07-6P**

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of cyclo[c]azepane derivs. for use as farnesyl transferase inhibitors)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 4 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:553089 HCAPLUS

DOCUMENT NUMBER: 137:109277

TITLE: Preparation of cycloheptenylaminomethylimidazoles as inhibitors of farnesyl protein transferase and geranylgeranyl protein transferase.

INVENTOR(S): Casara, Patrick; Le Diguarher, Thierry; Dorey, Gilbert; Hickman, John; Pierre, Alain; Tucker, Gordon; Guilbaud, Nicolas

PATENT ASSIGNEE(S): Les Laboratoires Servier S.A., Fr.

SOURCE: Eur. Pat. Appl., 28 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

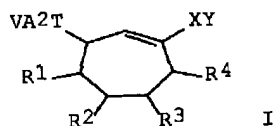
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1225170	A2	20020724	EP 2002-290101	20020116 <--
EP 1225170	A3	20020828		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
FR 2819509	A1	20020719	FR 2001-641	20010118 <--

FR 2819509	B1	20040416		
US 2002156113	A1	20021024	US 2002-50666	20020116
US 6638962	B2	20031028		
NO 2002000262	A	20020719	NO 2002-262	20020117 <--
CN 1365973	A	20020828	CN 2002-102042	20020117
BR 2002000114	A	20021022	BR 2002-114	20020117
NZ 516684	A	20030630	NZ 2002-516684	20020117
ZA 2002000471	A	20020722	ZA 2002-471	20020118 <--
AU 2002011937	A5	20020725	AU 2002-11937	20020118 <--
JP 2002265448	A2	20020918	JP 2002-9645	20020118
			FR 2001-641	A 20010118

PRIORITY APPLN. INFO.:  
OTHER SOURCE(S): MARPAT 137:109277  
GI



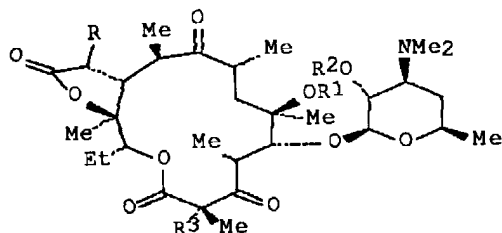
AB Title compds. [I; X = alkylene, CO, SO<sub>n</sub>, SO<sub>n</sub>Al, AlCOAl<sub>1</sub>, etc.; n = 0-2; Al, Al<sub>1</sub> = alkylene; Y = (substituted) aryl, heteroaryl, cycloalkyl, heterocycloalkyl; R<sub>1</sub>-R<sub>4</sub> = H, (substituted) aryl, heteroaryl, cycloalkyl, heterocycloalkyl; R<sub>1</sub>R<sub>2</sub>, R<sub>2</sub>R<sub>3</sub>, R<sub>3</sub>R<sub>4</sub> = bond, atoms to form (heterocyclic) rings; V = H, (substituted) aryl, heteroaryl; A<sub>2</sub> = (CR<sub>6</sub>R<sub>16</sub>)<sub>p</sub>; p = 0-4; R<sub>6</sub>, R<sub>16</sub> = H, alkyl, alkenyl, alkynyl, (substituted) aryl, heteroaryl, heterocycloalkyl, etc.; T = CHR<sub>5</sub>, NR<sub>5</sub>, NR<sub>5</sub>CO; R<sub>5</sub> = H, (substituted) alkyl, aryl, heteroaryl, aralkyl, heteroaryalkyl], were prepd. Thus, 3-(2-methylphenyl)-2-cyclohepten-1-ylamine (prepn. given), 4-[[5-formyl-1H-imidazol-1-yl)methyl]benzonitrile, and NaHB(OAc)<sub>3</sub> were stirred 48 h in dichloroethane to give 4-[[5-[[[3-(2-methylphenyl)-2-cyclohepten-1-yl]amino]methyl]-1H-imidazol-1-yl)methyl]benzonitrile. I inhibited FTPase and GGTase-1 with IC<sub>50</sub>'s in the nanomolar range and in the micromolar range, resp.

IT **443304-29-8P 443304-56-1P**  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of cycloheptenylaminomethylimidazoles as inhibitors of farnesyl protein transferase and geranylgeranyl protein transferase)

L30 ANSWER 5 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2002:487577 HCAPLUS  
DOCUMENT NUMBER: 137:63420  
TITLE: Preparation of lactone ketolide macrolide erythromycin antibiotics  
INVENTOR(S): Andreotti, Daniele; Arista, Luca; Biondi, Stefano; Cardullo, Francesca; Damiani, Frederica; Lociuoro, Sergio; Marchioro, Carla; Merlo, Giancarlo; Mingardi, Anna; Niccolai, Daniela; Paio, Alfredo; Piga, Elisabetta; Pozzan, Alfonso; Seri, Catia; Tarsi, Luca; Terreni, Silvia; Tibasco, Jessica  
PATENT ASSIGNEE(S): Glaxo Group Limited, UK  
SOURCE: PCT Int. Appl., 215 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002050091	A1	20020627	WO 2001-GB5665	20011220 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002017277	A5	20020701	AU 2002-17277	20011220 <--
EP 1363925	A1	20031126	EP 2001-271380	20011220
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NO 2003002846	A	20030820	NO 2003-2846	20030620
US 2004077557	A1	20040422	US 2003-450893	20031119
PRIORITY APPLN. INFO.:				
			GB 2000-31309	A 20001221
			GB 2001-26276	A 20011101
			GB 2001-26277	A 20011101
			WO 2001-GB5665	W 20011220

OTHER SOURCE(S): MARPAT 137:63420  
GI



I

AB The present invention relates to lactone ketolides I wherein R is H, CN, substituted alkyl; R1 is alkyl, alkenyl; R2 is H, hydroxy protecting group; R3 is H, halogen, and pharmaceutically acceptable salts and solvates thereof, to process for their prepn. and their use in therapy or prophylaxis of systemic or topical bacterial infections in a human or animal body. Thus, (11S,21R)-3-decladinoyl-11,12-dideoxy-6-O-methyl-3-oxo-12,11-[oxycarbonyl-(cyano)-methylene]erythromycin A was prepd. and tested as antibacterial agent against Streptococcus pneumoniae and Streptococcus pyogenes (MIC .ltoreq. 1 .mu.g/mL).

IT **439103-24-9P**

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

IT **245322-47-8**

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

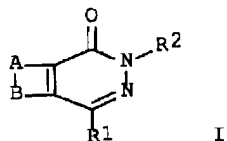
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 6 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2002:353439 HCAPLUS  
DOCUMENT NUMBER: 136:355242  
TITLE: Preparation of phthalazinones as PARP inhibitors  
INVENTOR(S): Martin, Niall Morrison Barr; Smith, Graeme Cameron  
Murray; White, Charles Richard; Newton, Roger Frank;  
Douglas, Diane Gillian; Eversley, Penny Jane; Vile,  
Julia  
PATENT ASSIGNEE(S): Kudos Pharmaceuticals Limited, UK; Maybridge PLC  
SOURCE: PCT Int. Appl., 109 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002036576	A1	20020510	WO 2001-GB4729	20011025 <--
W:				
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,				
PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,				
UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,				
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,				
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001095789	A5	20020515	AU 2001-95789	20011025 <--
EP 1330442	A1	20030730	EP 2001-976521	20011025
R:				
AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
GB 2384776	A1	20030806	GB 2003-9190	20011025
GB 2384776	B2	20040303		
BR 2001015062	A	20040217	BR 2001-15062	20011025
NZ 525138	A	20040326	NZ 2001-525138	20011025
JP 2004513121	T2	20040430	JP 2002-539335	20011025
US 2002183325	A1	20021205	US 2001-21506	20011030
NO 2003001498	A	20030402	NO 2003-1498	20030402
PRIORITY APPLN. INFO.:			GB 2000-26505	A 20001030
			US 2001-275066P	P 20010312
			US 2000-245662P	P 20001106
			WO 2001-GB4729	W 20011025

OTHER SOURCE(S): MARPAT 136:355242  
GI



AB The title compds. [I; A and B together represent (un)substituted fused arom. ring; R1 = LR3 (wherein L = (CH2)nQm(CH2)p; n, m, p = 0-3, the sum of n, m and p = 1-3; Q = O, S, NH, CO; R3 = (un)substituted C5-20 aryl); R2 = H, (un)substituted C1-7 alkyl, C3-20 heterocyclyl, C5-20 aryl, etc.],

useful for inhibiting the activity of PARP (poly(ADP-ribose)synthase), were prepd. General procedures for synthesis of I were described. Biol. data such as IC50 values against PARP, and DEF which is a ratio of the enhancement of the cell growth inhibition elicited by test compds. in the presence of bleomycin compared to bleomycin alone, were given. E.g., the compd. I [AB = benzo; R1 = 4-chlorobenzyl; R2 = H] showed IC50 of 1.8 .mu.M against PARP, and DEF of 1.9.

IT 420847-48-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of phthalazinones as PARP inhibitors)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 7 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:886056 HCAPLUS

DOCUMENT NUMBER: 136:15226

TITLE: Novel polyamine transport-inhibiting polyamine analogues as therapeutic and diagnostic agents

INVENTOR(S): Vermeulin, Nicolaas M. J.; O'day, Christine L.; Webb, Heather K.; Burns, Mark R.; Bergstrom, Donald E.

PATENT ASSIGNEE(S): Oridigm Corporation, USA

SOURCE: PCT Int. Appl., 102 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

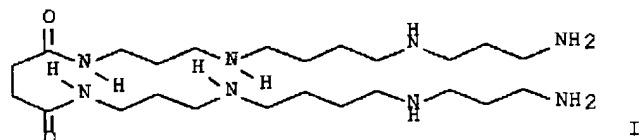
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001092218	A2	20011206	WO 2001-US17795	20010531 <--
WO 2001092218	A3	20030327		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6646149	B1	20031111	US 2000-584175	20000531
EP 1317424	A2	20030611	EP 2001-946044	20010531
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2004509845	T2	20040402	JP 2002-500833	20010531
PRIORITY APPLN. INFO.:			US 2000-584175	A 20000531
			US 1997-52586P	P 19970715
			US 1997-65728P	P 19971114
			US 1998-85538P	P 19980515
			WO 1998-US14896	A2 19980715
			US 1999-341400	A2 19990903
			US 1999-396523	A2 19990915
			WO 2001-US17795	W 20010531

GI

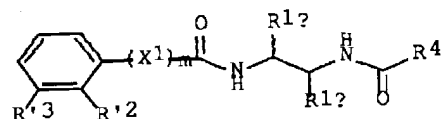


AB Novel "bispolyamine" inhibitor compds. of polyamine transport are disclosed. These compds. are useful pharmaceutical agents for treating diseases where it is desired to inhibit polyamine transport or other polyamine binding proteins, for example cancer and post-angioplasty injury. These compds. display desirable activities both for diagnostic and research assays and therapy. Most of the spermine dimers that have been tested provided very good Ki for transport inhibition with values under 75 nM. ORI 1236 (I) was the most potent inhibitor with a Ki of 22 nM. The results were generally mirrored in the growth inhibition assay. All of the compds. were synergistic with difluoromethylornithine, a polyamine synthesis inhibitor, with IC50 values of 10 .mu.M or less.

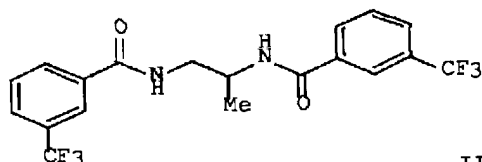
IT 220221-36-3  
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(novel polyamine transport-inhibiting polyamine analogs as therapeutic and diagnostic agents)

L30 ANSWER 8 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2001:472678 HCAPLUS  
DOCUMENT NUMBER: 135:76694  
TITLE: Synthesis and herbicidal efficacy of diacyl derivatives of propylene diamine  
INVENTOR(S): Hegde, Shridhar G.; Krupa, Daniel M.; Bohn, Joseph A.; Coffen, David L.; Gustafson, Gary R.; Kaplan, Alan P.; Ma, Yuting  
PATENT ASSIGNEE(S): Monsanto Co., USA  
SOURCE: PCT Int. Appl., 62 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046152	A1	20010628	WO 2000-US32937	20001205 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002052295	A1	20020502	US 2000-730529	20001205 <--
BR 2000016517	A	20020917	BR 2000-16517	20001205
PRIORITY APPLN. INFO.:			US 1999-172802P	P 19991221
			WO 2000-US32937	W 20001205
OTHER SOURCE(S):			MAREPAT 135:76694	
GI				



I



II

AB Compds. I are claimed [wherein; one of R1a and R1b = Me, CH2OH, or monohalomethyl and the other is hydrogen; X1 = CH2, O or S; m = 0 or 1; R'2 = H, halo or Me; R'3 = halo or halomethyl; R4 = .alpha.-halo or .alpha.,.alpha.-dihalo-alkyl or -(X2)n-R5, where X2 = CH2, O or S; n = 0 or 1; R5 = 5- or 6-membered (substituted) arom. or heterocyclic ring said ring optionally fused to a 5- or 6-membered (substituted) arom. or heterocyclic ring; with a proviso that no more than one ring substituent on the first and second 5- or 6-membered arom. or heterocyclic rings is other than a H, halo, Me, MeO or MeS]. Over 250 synthetic examples are provided. 1,2-Diaminopropane is acylated with 3-(trifluoromethyl)benzoyl chloride (THF, triethylamine, room temp.) to give diamide II in 73% yield. Compds. I were tested for herbicidal efficacy on 16 monocotyledonous and dicotyledonous plant species using a GR80 rating; the concn. at which 80% or greater inhibition obsd. In pre-emergence testing, II had GR80 = 65 - 1000 g/ha on most plant species. The (R)-enantiomer of II (III) was found to have GR80 values typically about one-half those of the racemic mixt. and the (S)-isomer was found to be inactive. Post-emergence testing was also conducted with compds. I. Pre-emergent field trials with III were said to exhibit acceptable control of several weed species (predominantly dicotyledonous) and was not injurious to corn, sorghum, or soybeans. Application of III in combination with .alpha.-chloroacetamides (e.g. acetochlor) showed greater control over plant species than with either of the herbicides alone indicating a synergistic interaction. A similar phenomena was obsd. for a selected compd. of the invention and glyphosate isopropylammonium salt in a post-emergence test.

IT 346669-13-4P 346669-15-6P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (synthesis and herbicidal efficacy of racemic and homochiral diacyl derivs. of propylene diamine)

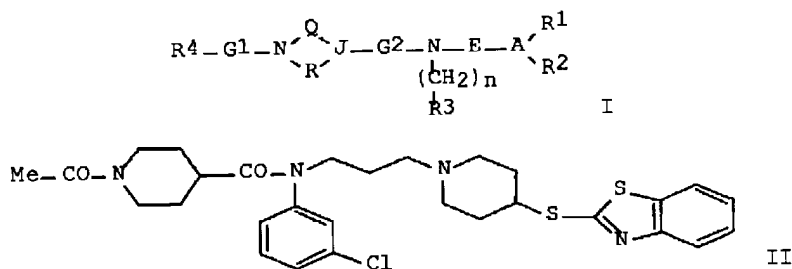
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 9 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2001:265385 HCAPLUS  
 DOCUMENT NUMBER: 134:295739  
 TITLE: Preparation of N-aryl-N-(heterocyclalkyl)piperidinecarboxamides as CCR5 antagonists  
 INVENTOR(S): Imamura, Shinichi; Hashiguchi, Shohei; Hattori, Taeko; Nishimura, Osamu; Kanzaki, Naoyuki; Baba, Masanori; Sugihara, Yoshihiro  
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan  
 SOURCE: PCT Int. Appl., 392 pp.  
 CODEN: PIXXD2

DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001025200	A1	20010412	WO 2000-JP6755	20000929 <--
W: AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000074487	A5	20010510	AU 2000-74487	20000929 <--
JP 2001302633	A2	20011031	JP 2000-302841	20000929 <--
BR 2000014428	A	20020611	BR 2000-14428	20000929 <--
EP 1220842	A1	20020710	EP 2000-962967	20000929 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003048880	A2	20030221	JP 2002-180545	20000929
NO 2002001450	A	20020603	NO 2002-1450	20020322 <--
US 6562978	B1	20030513	US 2002-89374	20020329
ZA 2002002593	A	20030403	ZA 2002-2593	20020403
US 2003114443	A1	20030619	US 2002-273111	20021018
PRIORITY APPLN. INFO.:				
			JP 1999-282088	A 19991001
			JP 2000-46749	A 20000218
			JP 2000-302841	A3 20000929
			WO 2000-JP6755	W 20000929
			US 2002-89374	A3 20020329

OTHER SOURCE(S): MARPAT 134:295739  
GI



AB Title compds. (I) [wherein R1 = H, (un)substituted hydrocarbon or nonarom. heterocycle; R2 = (un)substituted hydrocarbon or nonarom. heterocycle; or R1 and R2 together with A form an (un)substituted heterocycle; A = N or N+(R5).bul.Y-; R5 = hydrocarbon; Y- = counteranion; R3 = (un)substituted (hetero)cycle; n = 0 or 1; R4 = H or (un)substituted hydrocarbon, heterocycle, alkoxy, aryloxy, or amino group; E = (un)substituted divalent aliph. hydrocarbon; G1 = a bond, CO, or SO2; G2 = CO, SO2, NHCO, CONH, or OCO; J = CH or N; Q and R = independently a bond or (un)substituted divalent aliph. hydrocarbon; provided that J = CH when G2 = OCO, that 1 of Q and R is not a bond when the other is a bond, and that each of Q and R is not substituted by oxo group(s) when G1 is a bond; or a salt thereof]

were prepd. as potent chemokine receptor CCR5 antagonists. I are useful for the treatment or prevention of the HIV disease in humans (e.g. AIDS). For example, II.bul.HCl was synthesized in 34% yield in a 2-step process involving addn. of TFA to a soln. of 1-tert-butoxycarbonyl-4-(2-benzothiazolylthio)piperidine in CH<sub>2</sub>Cl<sub>2</sub>, followed by addn. of AcCN, 1-acetyl-N-(3-chlorophenyl)-N-(3-chloropropyl)-4-piperidinecarboxamide, K<sub>2</sub>CO<sub>3</sub>, and KI to the residue and workup. II.bul.HCl showed 96% inhibition of HIV-1 infection in transformant MAGI-CCR5 cells. In addn., 42 example compds. were tested and gave inhibition rates of 82% to 100% at 1.0 .mu.M in a CCR5 antagonistic activity assay.

IT **333990-73-1P**, N-(3,4-Dichlorophenyl)-N-[3-[4-(4-fluorobenzyl)-1-piperidinyl]propyl]-1-[2-(4-methylphenylthio)-3-pyridylcarbonyl]-4-piperidinecarboxamide trifluoroacetate (1:3)  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of N-aryl-N-(heterocyclalkyl)piperidinecarboxamide CCR5 antagonists by amidation of N-(arylheterocyclalkyl)alkylamines or addn. of heterocycles to N-aryl-N-(haloalkyl)piperidinecarboxamides)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 10 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:207925 HCAPLUS

DOCUMENT NUMBER: 134:237682

TITLE: Novel polyamine analogues as therapeutic and diagnostic agents

INVENTOR(S): Vermeulin, Nicholaas M. J.; O'Day, Christine L.; Webb, Heather K.; Burns, Mark R.; Bergstrom, Donald E.

PATENT ASSIGNEE(S): Oridigm Corporation, USA

SOURCE: Eur. Pat. Appl., 140 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1085011	A1	20010321	EP 2000-308049	20000915 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2001172244	A2	20010626	JP 2000-282752	20000918 <--
PRIORITY APPLN. INFO.:		US 1999-396523 A 19990915		

AB Novel inhibitors of polyamine transport having inhibition consts. two orders of magnitude lower than those of known compds. are disclosed. These polyamine analogs are useful pharmaceutical agents for treating disease where it is desired to inhibit polyamine transport or other polyamine binding proteins, for example cancer and post-angioplasty injury. Novel chem. synthetic methods to obtain polyamine analogs are disclosed, including the prodn. of a combinatorial polyamine library. These approaches yield analogs with desirable activities both for diagnostic and research assays and therapy. The assays of the invention are useful for high throughput screening of targets in the discovery of drugs that interact with the polyamine system.

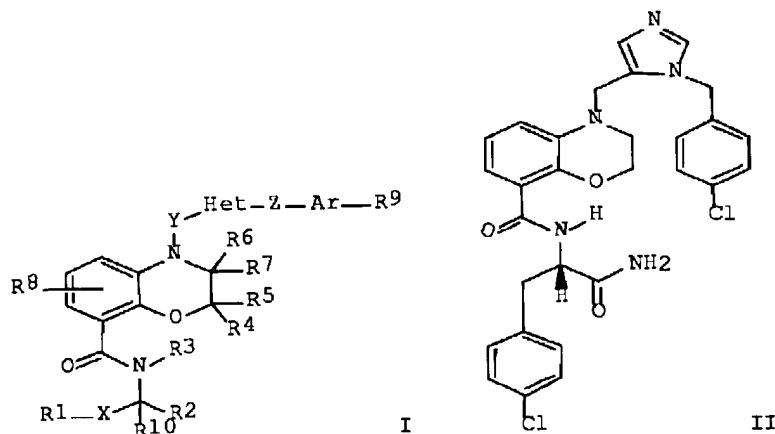
IT **220221-36-3P**

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of polyamines as therapeutic and diagnostic agents)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 11 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2001:101134 HCAPLUS  
 DOCUMENT NUMBER: 134:163045  
 TITLE: Preparation of benzoxazinecarboxamide derivatives as inhibitors of farnesyltransferase for the treatment of cancer  
 INVENTOR(S): Achard, Daniel; Jimonet, Patrick; Mailliet, Patrick; Sabuco, Jean-Francois  
 PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.  
 SOURCE: PCT Int. Appl., 127 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001009127	A1	20010208	WO 2000-FR2190	20000728 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG FR 2796943 A1 20010202 FR 1999-9894 19990730 <-- PRIORITY APPLN. INFO.: FR 1999-9894 A 19990730 OTHER SOURCE(S): MARPAT 134:163045 GI				



AB The invention concerns novel dihydro-8-benzoxazinecarboxamide derivs. I [R1 = alkyl, OH, alkoxy, hydroxyalkyl, (un)substituted (hetero)aryl; R2 = H, CO2H or derived radicals; R3 = H, (un)substituted alkyl; R4, R5 = H, alkyl; R6, R7 = H; or R6R7 = O; R8 = H, halo; R9 = H, halo, alkyl, (un)substituted (hetero)aryl, cycloalkyl, etc.; R10 = H, alkyl, alkoxy; X = (CH2)0-3; Y, Z = alkylene; Het = imidazole or pyridine nucleus; Ar = benzene nucleus] and their stereoisomers and salts. The compds. are

inhibitors of farnesyltransferase, and are useful against proliferative diseases, particularly in the treatment of cancer. The invention also concerns their prepn. and their use as therapeutic agents. For instance, Me 3-aminosalicylate underwent reductive alkylation with 1-(4-chlorobenzyl)-1H-imidazole-5-carboxaldehyde, followed by cyclization of the hydroxy amine with BrCH<sub>2</sub>CH<sub>2</sub>Br to form the benzoxazine ring. The ester function was hydrolyzed, the resultant acid then amidated with Me (L)-4-chlorophenylalaninate hydrochloride, and the reintroduced ester subjected to ammonolysis, to give title compd. II, isolated as the oxalate. Comps. I inhibited growth of human colon carcinoma cells HCT116 in vitro, with IC<sub>50</sub> values ranging from 0.1 nM to 100 .mu.M.

IT **325160-94-9P**, N-[1-(S)-Carbamoyl-2-(4-methoxyphenyl)ethyl]-4-[[3-(4-chlorobenzyl)-4-pyridyl]methyl]-3,4-dihydro-2H-benzo[b][1,4]oxazine-8-carboxamide **325162-05-8P**, N-[1-(S)-Carbamoyl-2-(4-methoxyphenyl)ethyl]-4-[[3-(4-chlorobenzyl)-4-pyridyl]methyl]-3,4-dihydro-2H-benzo[b][1,4]oxazine-8-carboxamide oxalate  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (drug candidate; prepn. of benzoxazinecarboxamide derivs. as inhibitors of farnesyltransferase for the treatment of cancer)

IT **325162-21-8P**, N-[1-(S)-Methoxycarbonyl-2-(4-methoxyphenyl)ethyl]-4-[[3-(4-chlorobenzyl)-4-pyridyl]methyl]-3,4-dihydro-2H-benzo[b][1,4]oxazine-8-carboxamide **325162-23-0P**, 4-[[3-(4-Chlorobenzyl)-4-pyridyl]methyl]-3,4-dihydro-2H-benzo[b][1,4]oxazine-8-carboxylic acid sodium salt **325162-26-3P**, 4-[[3-(4-Chlorobenzyl)-4-pyridyl]methyl]-3,4-dihydro-2H-benzo[b][1,4]oxazine-8-carboxylic acid methyl ester **325162-28-5P**, 3-[[[3-(4-Chlorobenzyl)-4-pyridyl]methyl]amino]salicylic acid methyl ester **325162-30-9P**, 3-[[[3-(4-Chlorobenzyl)-4-pyridyl]methylene]amino]salicylic acid methyl ester  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; prepn. of benzoxazinecarboxamide derivs. as inhibitors of farnesyltransferase for the treatment of cancer)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 12 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2000:814464 HCAPLUS  
 DOCUMENT NUMBER: 133:362712  
 TITLE: Preparation of quinoline derivatives as inhibitors of MEK enzymes  
 INVENTOR(S): Boyle, Francis Thomas; Gibson, Keith Hopkinson; Poyser, Jeffrey Philip; Turner, Paul  
 PATENT ASSIGNEE(S): Astrazeneca AB, Swed.  
 SOURCE: PCT Int. Appl., 187 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068201	A1	20001116	WO 2000-GB1697	20000503 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, IV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,				

DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,  
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
EP 1178967 A1 20020213 EP 2000-927491 20000503 <--  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO  
TR 200103186 T2 20020422 TR 2001-20010318620000503 <--  
BR 2000010391 A 20020702 BR 2000-10391 20000503 <--  
EE 200100589 A 20030217 EE 2001-589 20000503  
NZ 514980 A 20031031 NZ 2000-514980 20000503  
ZA 2001008971 A 20030130 ZA 2001-8971 20011030  
BG 106073 A 20020531 BG 2001-106073 20011101 <--  
NO 2001005448 A 20020107 NO 2001-5448 20011107 <--  
PRIORITY APPLN. INFO.: GB 1999-10577 A 19990508  
WO 2000-GB1697 W 20000503  
OTHER SOURCE(S): MARPAT 133:362712  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. [I; or a pharmaceutically acceptable salt thereof wherein: n is 0-1; X and Y are independently selected from NH, O, S, or NR8 where R8 is alkyl of 1-6 carbon atoms and X may addnl. comprise a CH2 group; R7 is a group (CH2)mR9 where m is 0, or an integer of from 1-3 and R9 is a substituted aryl group, an optionally substituted cycloalkyl ring of up to 10 carbon atoms, or an optionally substituted heterocyclic ring or an N-oxide of any nitrogen contg. ring; R6 is a divalent cycloalkyl of 3 to 7 carbon atoms, which may be optionally further substituted with one or more alkyl of 1 to 6 carbon atom groups; or is a divalent pyridinyl, pyrimidinyl, or Ph ring; wherein the pyridinyl, pyrimidinyl, or Ph ring may be optionally further substituted with one or more specified groups; R1, R2, R3 and R4 are each independently selected from hydrogen or various specified org. groups]. Title compds. are useful as pharmaceuticals for the inhibition of MEK activity. Thus, the title compd. II was prepd. and tested in HT29 human colon tumor cell proliferation assay.

IT 306999-01-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of quinoline derivs. as inhibitors of MEK enzymes)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 13 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:725622 HCAPLUS

DOCUMENT NUMBER: 133:296442

TITLE: Preparation of neurotrophic thio substituted pyrimidines

INVENTOR(S): Kelley, James L.; Krenitsky, Thomas A.; Beauchamp, Lilia M.

PATENT ASSIGNEE(S): Krenitsky Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 48 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000059893	A1	20001012	WO 2000-US9004	20000405 <--

W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN,  
CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB,  
GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ,  
LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ,  
PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ,  
UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,  
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,  
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

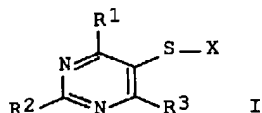
EP 1165522 A1 20020102 EP 2000-921705 20000405 <--

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO

PRIORITY APPLN. INFO.:

US 1999-127923P P 19990406  
US 1999-128842P P 19990412  
WO 2000-US9004 W 20000405

OTHER SOURCE(S): MARPAT 133:296442  
GI



AB The title compds. [I; R1 = NHR4 (R4 = aryl, alkyl, etc.), (un)substituted piperazino, homopiperazino, etc.; R2 = H, NH2; R3 = H; X = substituted aryl] and their pharmaceutically acceptable salts, useful in therapy, particularly in the treatment of neurodegenerative or other neurol. disorders of the central and peripheral systems, were prepd. and formulated. E.g., a multi-step synthesis of I [R1 = trans-4-hydroxycyclohexylamino; R2 = NH2; R3 = H; X = 4-ClC6H4] which doubled the ChAT activity over the activity with NGF alone at 0.04 .mu.M, was given.

IT 300855-81-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of neurotrophic thio substituted pyrimidines)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 14 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:725485 HCAPLUS

DOCUMENT NUMBER: 133:296658

TITLE: Preparation of desleucyl glycopeptide antibiotics

INVENTOR(S): Kahne, Daniel; Walker, Suzanne; Silva, Domingos J.

PATENT ASSIGNEE(S): The Trustees of Princeton University, USA; Incara Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 150 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

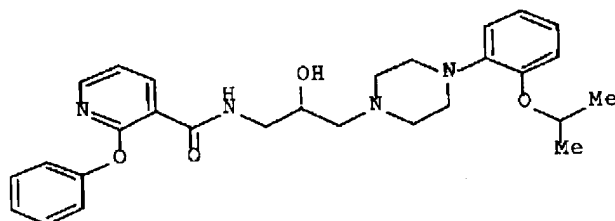
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000059528	A1	20001012	WO 2000-US8559	20000331 <--
W:				
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,				
CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,				
ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,				
LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,				

SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW,  
AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,  
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,  
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
EP 1173193 A1 20020123 EP 2000-919942 20000331 <--  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO  
US 6518243 B1 20030211 US 2000-540761 20000331  
US 1999-127516P P 19990402  
WO 2000-US8559 W 20000331  
PRIORITY APPLN. INFO.:  
AB Compds. that are analogs of glycopeptide antibiotics are disclosed. The  
compds. have the formula A1-A2-A3-A4-A5-A6-A7, where each of the groups A2  
to A7 is a modified or unmodified .alpha.-amino acid residue, A1 is  
optional and, when present, is an org. group other than N-substituted  
leucine, and at least one of the groups A1 to A7 is linked via a  
glycosidic bond to one or more glycosidic groups each having one or more  
sugar residues, where at least one of said sugar residues is modified to  
bear at least one hydrophobic substituent. Methods of making these  
compds., compns. including these compds., and methods of using the compds.  
to treat infections in a host are also disclosed. Antibacterial test data  
are tabulated for > 350 compds. of the invention.  
IT 300581-67-3P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of desleucyl glycopeptide antibiotics)  
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 15 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2000:619066 HCAPLUS  
DOCUMENT NUMBER: 134:424  
TITLE: Design, synthesis and biological evaluation of  
pyridine-phenylpiperazines: A novel series of potent  
and selective .alpha.1a-adrenergic receptor antagonist  
AUTHOR(S): Kuo, G.-H.; Prouty, C.; Murray, W. V.; Pulito, V.;  
Jolliffe, L.; Cheung, P.; Varga, S.; Evangelisto, M.;  
Shaw, C.  
CORPORATE SOURCE: Drug Discovery Division, The R.W. Johnson  
Pharmaceutical Research Institute, Raritan, NJ, 08869,  
USA  
SOURCE: Bioorganic & Medicinal Chemistry (2000),  
8(9), 2263-2275  
CODEN: BMECEP; ISSN: 0968-0896  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 134:424  
GI



I

AB Beginning from the screening hit and literature .alpha.1-adrenergic compds., a hybridized basic skeleton A was proposed as the pharmacophore for potent and selective .alpha.1a-AR antagonists. Introduction of a hydroxy group to increase the flexibility afforded B which served as the screening model and resulted in the identification of the second-generation lead 1. Using the Topliss approach, a no. of potent and selective .alpha.1a-AR antagonists were discovered. In all cases, binding affinity and selectivity at the .alpha.1a-AR of S-hydroxy enantiomers were higher than the R-hydroxy enantiomers. As compared to the des-hydroxy analogs, the S-hydroxy enantiomers displayed comparable potency and better selectivity at .alpha.1a-AR. The S-hydroxy enantiomer (I) (Ki=0.79 nM; =800; =104) was slightly less potent but much more selective at .alpha.1a-AR than tamsulosin (Ki=0.13 nM, =15, =1.4). I displayed higher selectivity in inhibiting rat prostate contraction over rat aorta contraction and also exhibited a higher degree of uroselectivity than tamsulosin in the anesthetized dog model.

IT 240418-34-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

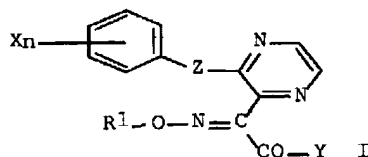
(design, synthesis and biol. evaluation of pyridinephenylpiperazines as a novel series of potent and selective .alpha.1a-adrenergic receptor antagonist)

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 16 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2000:139171 HCAPLUS  
DOCUMENT NUMBER: 132:180599  
TITLE: Preparation of phenoxy pyrazineacetic acid derivatives as agrochemical fungicides  
INVENTOR(S): Kusano, Nobuyuki; Eitsuka, Takayoshi; Niizeki, Yoshitaka  
PATENT ASSIGNEE(S): Kureha Chemical Industry Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 34 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000063362	A2	20000229	JP 1998-244408	19980814 <--
PRIORITY APPLN. INFO.:			JP 1998-244408	19980814
OTHER SOURCE(S):		MARPAT 132:180599		

GI



AB The title compds. I [R1 = H, alkyl; Y = alkoxy, etc.; X = H, halo, etc.; n = 0 - 5; Z = O, etc.] are prepd. The title compd. I [Xn = 3-Me; R1 = Me; Y = OMe; Z = O] at 1000 ppm gave 100% control of Puccinia recondita.

IT 259673-08-0P 259673-17-1P 259673-20-6P  
259673-23-9P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of phenoxyprazineacetic acid derivs. as agrochem. fungicides)

L30 ANSWER 17 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:686697 HCAPLUS

DOCUMENT NUMBER: 131:299463

TITLE: Preparation of heteroarylmethylpiperazinones and related compounds as inhibitors of farnesyl-protein transferase

INVENTOR(S): Wei, Dong D.; Williams, Theresa M.

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: U.S., 30 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

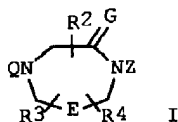
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5972942	A	19991026	US 1997-827485	19970327 <--
PRIORITY APPLN. INFO.:			US 1997-827485	19970327
OTHER SOURCE(S):		MARPAT 131:299463		

GI



AB Title compds. [I; Q = (R8)rVA1[C(R1a)2]nA2[C(R1a)2]n[W(R9)q]t[C(R1b)2]pX; R1a, R1b = H, aryl, heterocyclyl, cycloalkyl, alkenyl, alkynyl, (substituted) alkyl, etc.; R2, R3 = H, (substituted) alkyl, alkenyl, alkynyl, aryl, heterocyclyl, etc.; R2R3C = (CH2)u, etc.; R4 = H, Me; R8 = H, aryl, heterocyclyl, cycloalkyl, alkenyl, alkynyl, perfluoroalkyl, F, Cl, Br, (substituted) alkyl, etc.; R9 = H, alkenyl, alkynyl, perfluoroalkyl, F, Cl, Br, (substituted) alkyl, etc.; A1, A2 = bond, CH:CH2, C.tplbond.C, CO, O, imino, S, SO, SO2, etc.; E = (CH2)s; G = H2, O; V = H, heterocyclyl, aryl, alkyl, alkenyl, etc.; W = heterocyclyl; X = CH2, CO, S, SO, SO2; Z = (substituted) alkyl, cycloalkyl; n, p = 0-4; q = 1, 2; r = 0-5; s, t = 0, 1; with provisos], were prepd. Thus, 1-tert-butoxycarbonyl-2(S)-n-butyl-4-(2,2,2-trifluoroethyl)piperazin-5-one was stirred 1 h with CF3CO2H in CH2Cl2 to give a residue which was dissolved in dichloroethane and treated with N-methylmorpholine, Na(AcO)3BH, and 1-(4-cyanobenzyl)imidazolyl-5-carboxaldehyde followed by stirring overnight to give 2(S)-n-butyl-1-[1-(4-cyanobenzyl)-5-imidazolylmethyl]-4-(2,2,2-trifluoroethyl)piperazin-5-one dihydrochloride. I inhibited human FPTase with IC50.ltoreq.50 .mu.M.

IT 198084-17-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

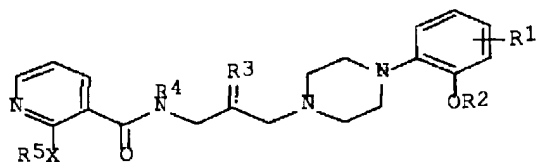
(prepn. of heteroarylmethylpiperazinones and related compds. as inhibitors of farnesyl-protein transferase)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS

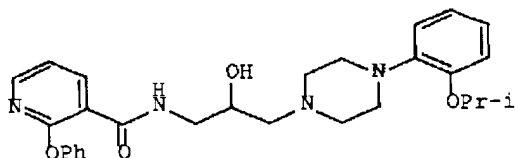
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 18 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1999:549258 HCAPLUS  
 DOCUMENT NUMBER: 131:184970  
 TITLE: Preparation of N-pyridinylcarbonylaminoalkyl-N'-arylpiperazines for treatment of benign prostatic hyperplasia.  
 INVENTOR(S): Kuo, Gee-Hong; Murray, William V.; Prouty, Catherine P.  
 PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA  
 SOURCE: PCT Int. Appl., 45 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9942448	A1	19990826	WO 1999-US3608	19990219 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
ZA 9901315	A	20001120	ZA 1999-1315	19990218 <--
US 6218396	B1	20010417	US 1999-252313	19990218 <--
AU 9933025	A1	19990906	AU 1999-33025	19990219 <--
AU 766398	B2	20031016		
BR 9909647	A	20001121	BR 1999-9647	19990219 <--
EP 1054868	A1	20001129	EP 1999-934281	19990219 <--
EP 1054868	B1	20030924		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, RO				
TR 200003220	T2	20010420	TR 2000-200003220	19990219 <--
JP 2002503724	T2	20020205	JP 2000-532400	19990219 <--
NZ 506462	A	20030725	NZ 1999-506462	19990219
CN 1121390	B	20030917	CN 1999-803027	19990219
AT 250580	E	20031015	AT 1999-934281	19990219
PT 1054868	T	20040130	PT 1999-934281	19990219
NO 2000004141	A	20001019	NO 2000-4141	20000818 <--
HK 1030776	A1	20040130	HK 2001-101679	20010308
PRIORITY APPLN. INFO.:				
US 1998-75321P P 19980220				
WO 1999-US3608 W 19990219				
OTHER SOURCE(S): MARPAT 131:184970				
GI				



I



II

AB Title compds. [I; R1 = H, halo, alkoxy, OH, alkyl; R2 = (substituted) alkyl, Ph, phenylalkyl; R3 = H, OH, alkoxy, O; R4 = H, alkyl, (substituted) phenylalkyl; R5 = (substituted) alkyl, Ph, phenylalkyl; X = O, S, NH; dotted line = optional double bond], were prepd. Thus, 1-(2-isopropoxyphenyl)piperazine was heated with 1-azido-3-tosyloxypropan-2-ol at 100.degree. for 36 h to give 76% 1-(2-isopropoxyphenyl)-4-(3-azido-2-hydroxypropyl)piperazine. The latter was hydrogenated in MeOH/aq. HCl over Pd/C at 50 psi for 16 h to give 95% amine, which was stirred with 2-phenoxy pyridine-3-carbonyl chloride, DMAP, and diisopropylethylamine in CH2Cl2 to give 69% title compd. (II). II inhibited norepinephrine-induced contractile response in aortic tissue and prostate tissue with IC50 = 4.74 .mu.M and 0.143 .mu.M, resp.

IT 240418-34-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of N-pyridinylcarbonylaminoalkyl-N'-arylpiperazines for treatment of benign prostatic hyperplasia)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 19 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:487274 HCAPLUS

DOCUMENT NUMBER: 131:116520

TITLE: Preparation of phenylalanine derivatives as pharmaceutical agents

INVENTOR(S): Head, John Clifford; Archibald, Sarah Catherine; Warrellow, Graham John; Porter, John Robert

PATENT ASSIGNEE(S): Celltech Therapeutics Limited, UK

SOURCE: PCT Int. Appl., 65 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9937618	A1	19990729	WO 1999-GB279	19990127 <--
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,			

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,  
CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
US 6329372 B1 20011211 US 1999-237060 19990126 <--  
AU 9924320 A1 19990809 AU 1999-24320 19990127 <--  
EP 1051399 A1 20001115 EP 1999-903798 19990127 <--  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, FI  
JP 2002501051 T2 20020115 JP 2000-528542 19990127 <--  
US 2002035127 A1 20020321 US 2001-964161 20010926 <--  
PRIORITY APPLN. INFO.: GB 1998-1674 A 19980127  
GB 1998-26669 A 19981203  
US 1999-237060 A1 19990126  
WO 1999-GB279 W 19990127

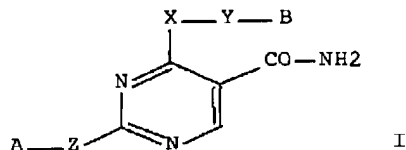
OTHER SOURCE(S): MARPAT 131:116520  
AB Phenylalanine derivs. 4-[R1(Alk1)rL1s]C6H2RaRb(Alk2)mCHRR2NR3COHet [R is a  
carboxylic acid or deriv.; R1 = H, OH, alkoxy or optionally substituted  
cycloaliph., polycycloaliph., heterocycloaliph., polyheterocycloaliph.,  
arom, or heteroarom. group; Alk1 = optionally substituted aliph. or  
heteroaliph. chain; L1 is a linker atom or group; r, s = 0, 1; Ra, Rb =  
-L2(CH2)pL3Rcq, where L2, L3 = a covalent bond or linker atom or group; p  
= 0, 1; q = 1-3; Rc = H, halo, alkyl, OH, alkoxy, etc.; Alk2 = alkylene; m  
= 0, 1; R2 = H, Me; R3 = H, alkyl; Het is an optionally substituted  
heteroarom. group] and their salts, solvates, hydrates and N-oxides were  
prepd. as pharmaceutical agents. Thus, N-(2-chloronicotinoyl)-N'-(3,5-  
dichloro-4-picoly)-L-4-aminophenylalanine was prepd. by coupling reaction  
of N-(3,5-dichloro-4-picoly)-L-4-aminophenylalanine Me ester with  
2-chloronicotinoyl chloride followed by ester hydrolysis. Title compds.  
were tested for inhibition of integrin-dependent cell adhesion and  
generally have IC50 values in the .alpha.4.beta.1 and .alpha.4.beta.7  
assays of 1.mu.M and below.

IT 232617-65-1P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of phenylalanine derivs. as pharmaceutical agents)  
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 20 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1999:404941 HCAPLUS  
DOCUMENT NUMBER: 131:44844  
TITLE: preparation of novel pyrimidine-5-carboxamide  
derivatives as tyrosinase inhibitors  
INVENTOR(S): Hisamichi, Hiroyuki; Naito, Ryo; Kawazoe, Souichirou;  
Toyoshima, Akira; Tanabe, Kazuhito; Nakai, Eiichi;  
Ichikawa, Atsushi; Orita, Akiko; Takeuchi, Makoto  
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan  
SOURCE: PCT Int. Appl., 43 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9931073	A1	19990624	WO 1998-JP5643	19981214 <--
W:	AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH,			
	GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,			
	LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI,			
	SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY,			
	KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,			

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,  
CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
AU 9915071 A1 19990705 AU 1999-15071 19981214 <--  
EP 1054004 A1 20001122 EP 1998-959197 19981214 <--  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI  
US 6432963 B1 20020813 US 2000-581595 20000615 <--  
PRIORITY APPLN. INFO.: JP 1997-344588 A 19971215  
WO 1998-JP5643 W 19981214  
OTHER SOURCE(S): MARPAT 131:44844  
GI



AB Pyrimidine-5-carboxamide derivs. or salts [I; X = O, S, NR1, CO, NR1CO, CONR1, C=NOR1, a bond; Y = lower alkylene optionally substituted by OR1 or NHR1, a bond; Z = O, NR2, a bond; A = H, optionally substituted lower alkyl, lower alkyl optionally having CO, optionally substituted aryl or heteroaryl, optionally substituted cycloalkyl, optionally substituted and satd. N heterocycle; B = optionally substituted aryl or heteroaryl; R1, R2 = H or lower alkyl optionally contg. CO], effective tyrosinase inhibitors useful as 5-HT antagonists, antiallergics, were prepd. I showed IC50 < 0.1 .mu.M in scintillation proximity assay. I were effective at 0.1-10 mg/kg-day p.o.

IT **227449-77-6P 227449-85-6P**  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of novel pyrimidine-5-carboxamide derivs. as tyrosinase inhibitors)

IT **227449-54-9P 227449-65-2P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. of novel pyrimidine-5-carboxamide derivs. as tyrosinase inhibitors)

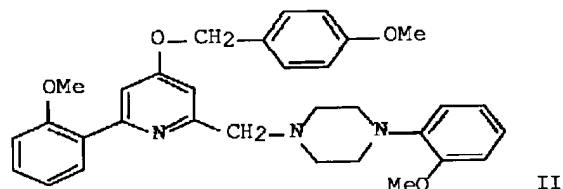
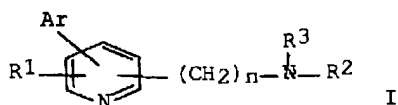
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 21 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1999:404931 HCAPLUS  
DOCUMENT NUMBER: 131:58848  
TITLE: Preparation of pyridine derivatives as 5-HT7 receptor binding agents  
INVENTOR(S): Adachi, Makoto; Sasatani, Takashi; Chomei, Nobuo; Fukui, Yoshikazu; Yasui, Mitsuru  
PATENT ASSIGNEE(S): Shionogi & Co., Ltd., Japan  
SOURCE: PCT Int. Appl., 146 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9931062	A1	19990624	WO 1998-JP5561	19981209 <--

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,  
DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,  
KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW,  
MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR,  
TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,  
FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,  
CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 9915045 A1 19990705 AU 1999-15045 19981209 <--  
PRIORITY APPLN. INFO.: JP 1997-347574 19971217  
WO 1998-JP5561 19981209  
OTHER SOURCE(S): MARPAT 131:58848  
GI



AB The title compds. I [Ar represents optionally substituted aryl or optionally substituted heteroaryl; R1 represents hydrogen, halogeno, alkyl, alkenyl, alkyloxy, etc.; R2 and R3 independently represent each hydrogen or optionally substituted alkyl or R2 and R3 may form together with the adjacent nitrogen atom an optionally substituted heterocycle; and n is an integer of 1 to 6] are prepd. In an in vitro test for 5-HT7 receptor binding, piperazinylmethylpyridine deriv. II showed the Ki value of 57 nM.

IT 228095-91-8P 228095-92-9P 228095-95-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of pyridine derivs. as 5-HT7 receptor binding agents)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 22 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:388161 HCAPLUS

DOCUMENT NUMBER: 131:58652

TITLE: Preparation of N-adamantylmethylbenzamides and analogs as purinergic P2Z receptor antagonists

INVENTOR(S): Baxter, Andrew; McInally, Thomas; Mortimore, Michael; Cladingboel, David

PATENT ASSIGNEE(S): Astra Pharmaceuticals Ltd., UK; Astra Aktiebolag

SOURCE: PCT Int. Appl., 86 pp.

CODEN: PIXXD2

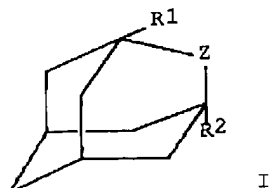
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9929661	A1	19990617	WO 1998-SE2188	19981201 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2312420	AA	19990617	CA 1998-2312420	19981201 <--
AU 9917913	A1	19990628	AU 1999-17913	19981201 <--
AU 744280	B2	20020221		
EP 1036059	A1	20000920	EP 1998-962751	19981201 <--
EP 1036059	B1	20020918		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9813390	A	20001003	BR 1998-13390	19981201 <--
TR 200001605	T2	20001023	TR 2000-200001605	19981201 <--
JP 2001525392	T2	20011211	JP 2000-524258	19981201 <--
EE 200000378	A	20011217	EE 2000-200000378	19981201 <--
AT 224360	E	20021015	AT 1998-962751	19981201
PT 1036059	T	20030228	PT 1998-962751	19981201
ES 2184352	T3	20030401	ES 1998-962751	19981201
RU 2214997	C2	20031027	RU 2000-117574	19981201
US 6201024	B1	20010313	US 1999-230478	19990126 <--
NO 2000002786	A	20000731	NO 2000-2786	20000531 <--
US 2001003121	A1	20010607	US 2000-745740	20001226 <--
US 6303659	B2	20011016		
US 6258838	B1	20010710	US 2000-745346	20001226 <--
PRIORITY APPLN. INFO.:				
			SE 1997-4544	A 19971205
			WO 1998-2188	W 19981201
			WO 1998-SE2188	W 19981201
			US 1999-230478	A1 19990126
OTHER SOURCE(S):			MARPAT 131:58652	
GI				



AB Title compds. [I; R1 = (CH<sub>2</sub>)<sub>x</sub>NHCOR; R = (un)substituted Ph, -pyridyl, -indolyl, etc.; R2 = H or halo; Z = O or CH<sub>2</sub>; X = 1 or 2] were prepd. Thus, 1-adamantanemethylamine was amidated by 2,4-Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>COCl to give I (R1 = CH<sub>2</sub>NHCOC<sub>6</sub>H<sub>3</sub>Cl<sub>2</sub>-2,4, R2 = H, Z = CH<sub>2</sub>). Data for biol. activity of I were given.

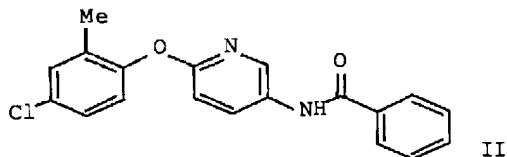
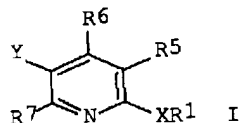
IT 227327-50-6P 227327-73-3P 227327-80-2P  
227327-82-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of N-adamantylmethylbenzamides and analogs as purinergic P2Z

receptor antagonists)  
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 23 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1999:325908 HCAPLUS  
DOCUMENT NUMBER: 130:352186  
TITLE: Substituted pyridine compounds as anti-inflammatory  
agents  
INVENTOR(S): Mantlo, Nathan B.; Schlachter, Steven T.; Josey, John  
A.  
PATENT ASSIGNEE(S): Amgen Inc., USA  
SOURCE: PCT Int. Appl., 254 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9924404	A1	19990520	WO 1998-US23510	19981104 <--
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6022884	A	20000208	US 1998-185119	19981103 <--
CA 2307552	AA	19990520	CA 1998-2307552	19981104 <--
AU 9913065	A1	19990531	AU 1999-13065	19981104 <--
AU 742442	B2	20020103		
EP 1028945	A1	20000823	EP 1998-956570	19981104 <--
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
JP 2001522834	T2	20011120	JP 2000-520418	19981104 <--
US 6184237	B1	20010206	US 1999-431410	19991101 <--
US 6333341	B1	20011225	US 2000-642860	20000821 <--
US 2002035094	A1	20020321	US 2001-932281	20010817 <--
US 6458813	B2	20021001		
PRIORITY APPLN. INFO.:			US 1997-64953P	P 19971107
			US 1998-185119	A 19981103
			WO 1998-US23510	W 19981104
			US 1999-431410	A3 19991101
			US 2000-642860	A3 20000821
OTHER SOURCE(S):		CASREACT 130:352186; MARPAT 130:352186		
GI				



AB Title compds. [I; wherein X is O, S, S(O), S(O)<sub>2</sub> or NR<sub>2</sub>; Y is -C(O)-NR<sub>3</sub>R<sub>4</sub> or -NR<sub>4</sub>-C(O)-R<sub>3</sub>; R<sub>1</sub> is a cycloalkyl, aryl, heterocyclyl or heteroaryl radical which is optionally substituted by 1-4 radicals of alkyl, halo, haloalkyl, cyano, azido, nitro, amidino, R<sub>18</sub>-Z<sub>18</sub>- or R<sub>18</sub>-Z<sub>18</sub>-alkyl; provided that the total no. of aryl, heteroaryl, cycloalkyl and heterocyclyl radicals in R<sub>1</sub> is 1-3; and provided when Y is -NR<sub>4</sub>-C(O)-R<sub>3</sub> and X is O or S, R<sub>1</sub> is other than a 2-pyrimidinyl radical; R<sub>2</sub> is a hydrogen or alkyl radical; R<sub>3</sub> is an aryl or heteroaryl radical which is optionally substituted by 1-5 radicals of alkyl, halo, haloalkyl, cyano, azido, nitro, amidino, R<sub>19</sub>-Z<sub>19</sub>- or R<sub>19</sub>-Z<sub>19</sub>-alkyl; provided that the total no. of aryl and heteroaryl radicals in R<sub>3</sub> is 1-3; and provided when Y is -C(O)-NR<sub>3</sub>R<sub>4</sub>, R<sub>3</sub> is other than a Ph or naphthyl having an amino, nitro, cyano, carboxy or alkoxycarbonyl] or a pharmaceutically acceptable salt thereof, are prepd. and effective for prophylaxis and treatment of diseases, such as TNF- $\alpha$ , IL-1 $\beta$ , IL-6 and/or IL-8 mediated diseases, and other maladies, such as pain and diabetes. The invention encompasses novel compds., analogs, prodrugs and pharmaceutically acceptable salts thereof, pharmaceutical compns. and methods for prophylaxis and treatment of diseases and other maladies or conditions involving inflammation, pain, diabetes, cancer and the like. The subject invention also relates to processes for making such compds. as well as to intermediates useful in such processes or a pharmaceutically acceptable salt thereof.

IT 224798-42-9P 224799-37-5P 224800-84-4P  
224801-77-8P 224802-65-7P 224803-75-2P  
224804-80-2P 224805-72-5P 224806-63-7P  
224807-56-1P 224808-46-2P 224809-64-7P  
224810-57-5P 224811-52-3P 224812-92-4P  
224813-98-3P 224814-98-6P 224822-03-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted pyridines as anti-inflammatory agents)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 24 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:205309 HCAPLUS

DOCUMENT NUMBER: 130:237591

TITLE: Preparation of piperazinones as inhibitors of farnesyl-protein transferase

INVENTOR(S): Dinsmore, Christopher J.

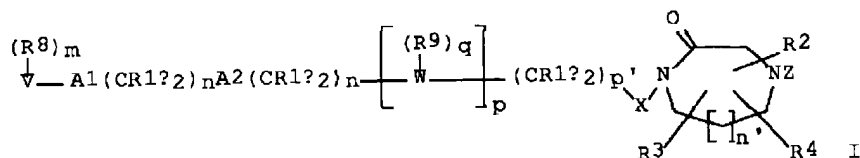
PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: U.S., 28 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5885995	A	19990323	US 1997-827482	19970327 <--
PRIORITY APPLN. INFO.:			US 1997-827482	19970327
OTHER SOURCE(S):	MARPAT 130:237591			
GI				



AB The title compds. I [R1a, R1b = H, aryl, cycloalkyl, etc.; R2, R3 = H, alkyl, alkenyl, etc.; CH2 = H, Me; R8 = H, aryl, perfluoroalkyl, etc.; R9 = H, alkenyl, alkynyl, F, Cl, etc.; A1, A2 = bond, CH:CH, C.tplbond.C, etc.; V = H, aryl, alkyl, alkenyl; W = pyridinyl, imidazolyl; Z = aryl, arylmethyl, arylsulfonyl, etc.; m = 1; n = 0-4; p = 1; q = 1, 2; p' = 0-4; n' = 0], which inhibit farnesyl-protein transferase (FTase) and the farnesylation of the oncogene protein Ras, were prepd. E.g., 4-(3-chlorophenyl)-1-[1-(4-cyanobenzyl)-5-imidazolylmethyl]-2-piperazinone hydrochloride was prepd.

IT 197853-30-8P 197853-33-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of piperazinones as inhibitors of farnesyl-protein transferase)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 25 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:77533 HCAPLUS

DOCUMENT NUMBER: 130:153469

TITLE: Novel polyamine analogs as therapeutic and diagnostic agents

INVENTOR(S): Vermeulin, Nicolaas M. J.; O'Day, Christine L.; Webb, Heather K.; Burns, Mark R.; Bergstrom, Donald E.

PATENT ASSIGNEE(S): Oridigm Corporation, USA

SOURCE: PCT Int. Appl., 143 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

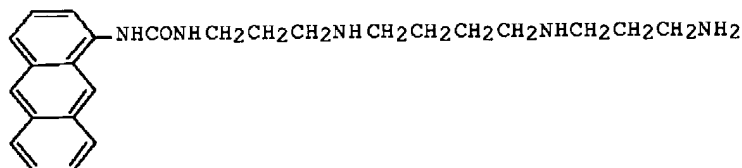
FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9903823	A2	19990128	WO 1998-US14896	19980715 <--
WO 9903823	A3	19990408		
W:	AL, AM, AU, AZ, BA, BB, BG, BR, CA, CN, CU, CZ, EE, FI, GE, HU, IL, IS, JP, KG, KP, KR, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,			

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,  
CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
AU 9884968 A1 19990210 AU 1998-84968 19980715 <--  
AU 758570 B2 20030327  
EP 1001927 A2 20000524 EP 1998-935790 19980715 <--  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, FI  
JP 2001510181 T2 20010731 JP 2000-503054 19980715 <--  
US 6172261 B1 20010109 US 1999-341400 19990903 <--  
US 6646149 B1 20031111 US 2000-584175 20000531  
PRIORITY APPLN. INFO.: US 1997-52586P P 19970715  
US 1997-65728P P 19971114  
US 1998-85538P P 19980515  
WO 1998-US14896 W 19980715  
US 1999-341400 A2 19990903  
US 1999-396523 A2 19990915

OTHER SOURCE(S): MARPAT 130:153469  
GI



I

AB Title inhibitors RXR1 [ R =H, or is a head group consisting of a straight or branched C1-10 aliph., alicyclic, single or multiring arom., single or multiring aryl substituted aliph., etc.; R1 is a polyamine; X = CO, NHCO, NHCS, SO2] and pharmaceutical acceptable salts of polyamine transport having inhibition consts. two orders of magnitude lower than those of known compds. are disclosed. These polyamine analogs are useful pharmaceutical agents for treating diseases where it is desired to inhibit polyamine transport or other polyamine binding proteins, for example cancer and post-angioplasty injury and the introduction of a 3-amidopropyl group to the diaminobutyl part of spermidine produce a significantly better transport inhibitor. Novel chem. synthetic methods to obtain polyamine analogs are disclosed, including the prodn. of a combinatorial polyamine library. These approaches yield analogs with desirable activities both for diagnostic and research assays and therapy. The assays of the invention are useful for high throughput screening of targets in the discovery of drugs that interact with the polyamine system. Thus, I was prepd. from 1-aminoanthracene, 4-nitrophenyl chloroformate, and spermine.

IT 220221-36-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(prepn. of polyamines as therapeutic and diagnostic agents)

L30 ANSWER 26 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:45145 HCAPLUS

DOCUMENT NUMBER: 130:125091

TITLE: Preparation of piperazine-2,3-dione derivatives as inhibitors of farnesyl-protein transferase

INVENTOR(S): Dinsmore, Christopher J.; Williams, Theresa M.

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

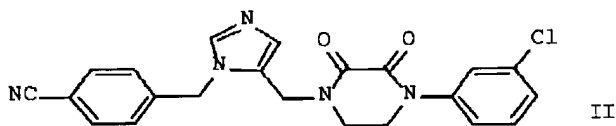
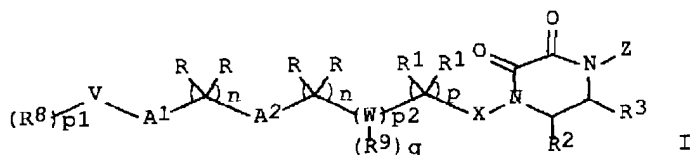
SOURCE: U.S., 29 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5859012	A	19990112	US 1997-823923	19970325 <--
PRIORITY APPLN. INFO.:			US 1997-823923	19970325
OTHER SOURCE(S):	MARPAT 130:125091			
GI				



AB The invention is directed to piperazine-2,3-dione compds. I [A1, A2 = bond, CH:CH, C.tplbond.C, CO, (un)substituted CONH, NHCO, O, NH, S, S(O), SO2, etc.; R, R1 = H, aryl, cycloalkyl, alkenyl, alkynyl, cyano, NO2, N3, (un)substituted OH, (un)substituted NH2, (un)substituted alkyl, etc.; R2, R3 = H, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted aryl, (un)substituted carbamoyl, (un)substituted CO2H; R8 = H, aryl, cycloalkyl, alkenyl, alkynyl, perfluoroalkyl, F, Cl, Br, (un)substituted OH, (un)substituted CONH2, cyano, NO2, N3, (un)substituted alkyl, etc.; R9 = H, alkenyl, alkynyl, perfluoroalkyl, F, Cl, Br, (un)substituted OH, (un)substituted CONH2, cyano, NO2, N3, (un)substituted NH2, (un)substituted alkyl, etc.; V = H, aryl, alkenyl, alkyl with 0-4 C atoms replaced by O, S, or N; W = imidazole; X = bond, CH2, CO, S, SO, SO2; Z = (un)substituted aryl, arylmethyl, (un)substituted arylsulfonyl, (un)substituted alkyl, or (un)substituted cycloalkyl, etc.; n, p = 0-4; q = 1, 2; p1 = 0-5, provided that p1 = 0 when V = H; p2 = 1], which inhibit farnesyl-protein transferase (FPTase) and the farnesylation of the oncogene protein Ras. The invention is further directed to chemotherapeutic compns. contg. the invention compds., and methods for inhibiting FPTase and the farnesylation of the oncogene protein Ras. The compds. have application as antitumor agents, and are also useful or potentially useful for treating other proliferative diseases, viral infections, restenosis, polycystic kidney disease, and fungal infections. Thus, 1-(4-cyanobenzyl)-5-imidazolecarboxaldehyde was added to a mixt. of NaBH(OAc)3, Me N-(2-aminoethyl)-N-(3-chlorophenyl)oxalamide hydrochloride, and 4.ANG. mol. sieves at 0.degree., and the mixt. was stirred at room temp. overnight to give, after salt formation with HCl, the title compd. II.HCl. Several title compds., including II, inhibited human FPTase in vitro with IC50 of .ltoreq. 10 .mu.M.

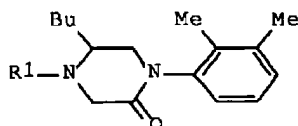
IT 219919-15-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(target compd.; prepn. of piperazinedione derivs. as inhibitors of farnesyl protein transferase)

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 27 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1999:34471 HCAPLUS  
DOCUMENT NUMBER: 130:95565  
TITLE: Preparation of 1-aryl(carbonyl)-2-piperazinones and analogs as farnesyl protein transferase inhibitors  
INVENTOR(S): Anthony, Neville J.; Ciccarone, Terrence M.; Dinsmore, Christopher J.; Gomez, Robert P.; Williams, Theresa M.; Hartman, George D.  
PATENT ASSIGNEE(S): Merck and Co., Inc., USA  
SOURCE: U.S., 68 pp., Cont.-in-part of U.S. Ser. No. 470,690, abandoned.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5856326	A	19990105	US 1996-600728	19960301 <--
CA 2216707	AA	19961003	CA 1996-2216707	19960325 <--
WO 9630343	A1	19961003	WO 1996-US4019	19960325 <--
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, US, US, UZ, VN, AM, AZ, BY, KG				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9653223	A1	19961016	AU 1996-53223	19960325 <--
AU 710672	B2	19990923		
EP 820445	A1	19980128	EP 1996-909851	19960325 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI				
BR 9607953	A	19980714	BR 1996-7953	19960325 <--
CN 1195340	A	19981007	CN 1996-194206	19960325 <--
JP 10511098	T2	19981027	JP 1996-529559	19960325 <--
JP 3043815	B2	20000522		
ZA 9602433	A	19961002	ZA 1996-2433	19960327 <--
NO 9704457	A	19971128	NO 1997-4457	19970926 <--
PRIORITY APPLN. INFO.:			US 1995-412829	B2 19950329
			US 1995-470690	B2 19950606
			US 1996-600728	A 19960301
			WO 1996-US4019	W 19960325
OTHER SOURCE(S):		MARPAT 130:95565		
GI				



II

AB R1A1Z1A2Z2Z3Z4XZR [I; A1,A2 = bond, O, CO, CH:CH, etc.; R = (un)substituted heterocyclylcarbonyl or -arylcarbonyl when Z = e.g.,

(un)substituted 1,4-piperazinediyl; R = (un)substituted (hetero)aryl(methyl) or -(sulfonyl) when Z = e.g., (un)substituted 3-oxopiperazine-1,4-diyl; R1 = H, alkyl, aryl, etc.; X = CH2, CO, SOO-2; Z1,Z2,Z4 = bond or (un)substituted alkylene; Z3 = bond or (un)substituted heterocyclylene] were prep'd. Thus, (S)-BuCH(NHCO2CMe3)CO2H was amidated by MeONHMe and the reduced product reductively aminated by 2,3-Me2C6H3NH2 to give, after cyclocondensation with ClCH2COCl, arylpiperazinone (S)-II (III; R1 = H) which was deprotected and the product reductively condensed with 1-triphenylmethylimidazole-4-carboxaldehyde to give, after deprotection, III (R1 = 4-imidazolylmethyl). Data for biol. activity of I were given.

IT 219552-94-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of 1-aryl(carbonyl)-2-piperazinones and analogs as farnesyl protein transferase inhibitors)

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 28 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:479031 HCAPLUS

DOCUMENT NUMBER: 129:122662

TITLE: Preparation of imidazole derivatives as inhibitors of farnesyl-protein transferase

INVENTOR(S): Bergman, Jeffrey; Dinsmore, Christopher

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: U.S., 21 pp.  
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5780488	A	19980714	US 1997-824588	19970326 <--
PRIORITY APPLN. INFO.:			US 1997-824588	19970326

OTHER SOURCE(S): MARPAT 129:122662

AB The title compds. (R6)rVAL(CR1a2)nA2(C1b2)n(WR7)t(CR22)pA3(CR22)pXR3R4 [R1a, R1b, R2 = H, aryl, heterocyclyl, etc.; R3, R4 = H, F, Cl, etc.; A3 = NR5S(O)m, etc.; m = 0 - 2; R5 = H, (un)substituted aryl, etc.; R6, R7 = H, aryl, heterocyclyl, etc.; A1, A2 = bond, CH:CH, etc.; X = aryl, heteroaryl; V = H, heterocyclyl, etc.; W = heterocyclyl; n, p = 0 - 4; r = 0 - 5, provided that r is 0 when V is hydrogen, and t is 1], useful as farnesyl-protein transferase inhibitors (no data), are prep'd. The present invention is directed to compds. which inhibit farnesyl-protein transferase (FTase) and the farnesylation of the oncogene protein Ras. The invention is further directed to chemotherapeutic compns. contg. the compds. of this invention and methods for inhibiting farnesyl-protein transferase and the farnesylation of the oncogene protein Ras.

IT 197786-21-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of imidazole derivs. as inhibitors of farnesyl-protein transferase)

IT 197786-45-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. of imidazole derivs. as inhibitors of farnesyl-protein transferase)

IT 197786-28-0 197786-35-9

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(prepn. of imidazole derivs. as inhibitors of farnesyl-protein  
transferase)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 29 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:115356 HCAPLUS

DOCUMENT NUMBER: 128:154011

TITLE: Preparation of 9-thioxanthenecarboxamides and  
9-fluorencarboxamides as inhibitors of microsomal  
triglyceride transfer protein

INVENTOR(S): Biller, Scott A.; Dickson, John K.; Lawrence, R.  
Michael; Magnin, David R.; Poss, Michael A.; Robl,  
Jeffrey A.; Sulsky, Richard B.; Tino, Joseph A.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA

SOURCE: U.S., 98 pp., Cont.-in-part of U. S. Ser. No.472,067.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

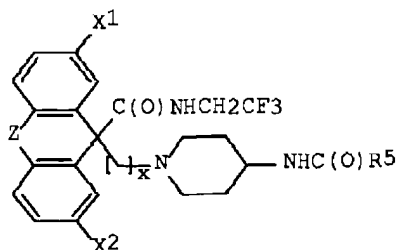
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5712279	A	19980127	US 1996-548811	19960111 <--
CA 2091102	AA	19930907	CA 1993-2091102	19930305 <--
HU 67962	A2	19950529	HU 1993-627	19930305 <--
HU 218419	B	20000828		
JP 06038761	A2	19940215	JP 1993-46499	19930308 <--
EP 584446	A2	19940302	EP 1993-103697	19930308 <--
EP 584446	A3	19950426		
EP 584446	B1	20020619		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
AT 219514	E	20020715	AT 1993-103697	19930308 <--
PT 584446	T	20020930	PT 1993-103697	19930308
ES 2178640	T3	20030101	ES 1993-103697	19930308
AU 670930	B2	19960808	AU 1993-34064	19930309 <--
AU 9334064	A1	19930909		
US 5739135	A	19980414	US 1995-472067	19950606 <--
ZA 9601340	A	19970911	ZA 1996-1340	19960220 <--
LT 4367	B	19980825	LT 1997-152	19970919 <--

PRIORITY APPLN. INFO.:

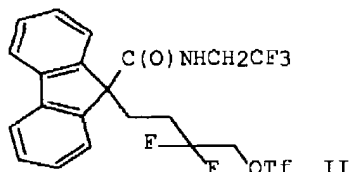
US 1995-391901	B2	19950221
US 1995-472067	A2	19950606
US 1992-847503	A	19920306
US 1993-117362	A2	19930903
US 1994-284808	B2	19940805

OTHER SOURCE(S): MARPAT 128:154011

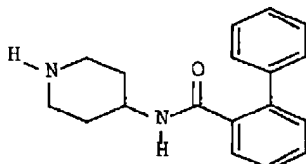
GI



I



II



III

AB The title compds. [I; Z = a bond, S; X1, X2 = H, halo; x = 2-6; (CH2)x is optionally substituted with 1-3 substituents such as alkyl or halo; R5 = (un)substituted heteroaryl, aryl, heterocycloalkyl, cycloalkyl] and their piperidine N-oxides, which inhibit microsomal triglyceride transfer protein and thus are useful for preventing or treating atherosclerosis, pancreatitis secondary to hypertriglyceridemia, hyperglycemia, or obesity, and for lowering serum lipid levels, or preventing and/or treating hyperlipemia, hyperlipidemia, hyperlipoproteinemia, hypercholesterolemia, and/or hypertriglyceridemia, were prepd. Thus, reaction of 9-fluorene-9-carboxamide II (prepn. of both reagents is described) with piperidine III in PhMe/DMF afforded the title compd. I [Z = a bond; X1 = X2 = H; (CH2)x = (CH2)2CF2CH2; R5 = 2-biphenyl]. Compds. I are effective at 5-500 mg/day.

IT 182432-31-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of 9-thioxanthenecarboxamides and 9-fluorene-9-carboxamides as inhibitors of microsomal triglyceride transfer protein)

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 30 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:679076 HCAPLUS

DOCUMENT NUMBER: 127:331505

TITLE: Preparation of 1-imidazolylmethyl-4-phenylpiperazine-2,3-diones and analogs as farnesyl protein transferase inhibitors

INVENTOR(S): Dinsmore, Christopher J.; Williams, Theresa M.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Dinsmore, Christopher J.; Williams, Theresa M.

SOURCE: PCT Int. Appl., 105 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

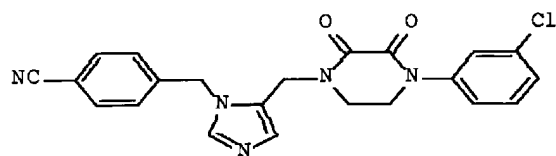
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9736889	A1	19971009	WO 1997-US5058	19970327 <--

W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU,

IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX,  
NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN,  
YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB,  
GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN,  
ML, MR, NE, SN, TD, TG  
CA 2250190 AA 19971009 CA 1997-2250190 19970327 <--  
AU 9725930 A1 19971022 AU 1997-25930 19970327 <--  
AU 716338 B2 20000224  
EP 891350 A1 19990120 EP 1997-917667 19970327 <--  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI  
JP 2000507580 T2 20000620 JP 1997-535440 19970327 <--  
PRIORITY APPLN. INFO.: US 1996-14589P P 19960403  
GB 1996-14315 A 19960708  
WO 1997-US5058 W 19970327  
OTHER SOURCE(S): MARPAT 127:331505  
GI



II

AB R1A1[C(R1a)2]nA2[C(R1a)2]nZ[C(R1b)2]pZ1Z2R [I; A1,A2 = bond, CH:CH, CO, O, CONH, etc.; R = (un)substituted (cyclo)alkyl, -(hetero)aryl(methyl), -(hetero)arylsulfonyl; R1 = H, (un)substituted heterocyclyl, -aryl, -alk(en)yl; R1a,R1b = H, alkyl, acyl, heterocyclyl, aryl, etc.; Z = bond or (un)substituted heterocyclylene; Z1 = bond, CH2, CO, SOO-2; Z2 = (un)substituted 2,3-dioxopiperazine-1,4-diyl; n,p = 0-4] were prepd. Thus, 1-trityl-4-acetoxymethylimidazole (prepn. given) was condensed with BrCH2C6H4(CN)-4 and the deprotected product oxidized to give 1-(4-cyanobenzyl)imidazole-5-carboxaldehyde which was cyclocondensed with 3-ClC6H4N(COCO2Me)CH2CH2NH2.HCl (prepn. given) to give title compd. II.HCl. Data for biol. activity of I were given.  
IT 197912-97-3P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of 1-imidazolylmethyl-4-phenylpiperazine-2,3-diones and analogs as farnesyl protein transferase inhibitors)

L30 ANSWER 31 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:679075 HCAPLUS

DOCUMENT NUMBER: 127:331509

TITLE: preparation of piperazine-2,5-dione derivs. as inhibitors of farnesyl-protein transferase

INVENTOR(S): Dinsmore, Christopher J.; Williams, Theresa M.; Bergman, Jeffrey

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Dinsmore, Christopher J.; Williams, Theresa M.; Bergman, Jeffrey

SOURCE: PCT Int. Appl., 96 pp.

CODEN: PIXXD2

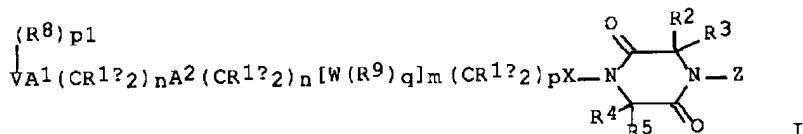
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9736888	A1	19971009	WO 1997-US4711	19970327 <--
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5919785	A	19990706	US 1997-823921	19970325 <--
CA 2249604	AA	19971009	CA 1997-2249604	19970327 <--
AU 9725875	A1	19971022	AU 1997-25875	19970327 <--
AU 715667	B2	20000210		
EP 891349	A1	19990120	EP 1997-917599	19970327 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2000507576	T2	20000620	JP 1997-535347	19970327 <--
PRIORITY APPLN. INFO.:				
			US 1996-14587P	P 19960403
			GB 1996-13461	A 19960627
			WO 1997-US4711	W 19970327
OTHER SOURCE(S): MARPAT 127:331509				
GI				



AB The invention relates to substituted piperazine-2,5-diones I (R1a = H, C1-C6 alkyl; R1b = H, aryl, heterocycle, etc.; R2 = H, aryl, etc.; R3 = H, CH3, etc.; R4 = H, aryl, etc.; R8 = H, aryl, heterocycle, CN, NO2, etc.; A1 = CO, CH:CH, O, etc.; A2 = CO, CH:CH, O, etc.; V = H, aryl, alkyl, etc.; W = heterocycle; X = CH2, CO, bond, etc.; Z = Aryl, arylmethyl, arylsulfonyl, etc.; m = 0, 1; n = 0-4; p = 0-4; q = 1, 2; p1 = 0-5) and a pharmaceutically acceptable salt thereof, that inhibit farnesyl-protein transferase and ras protein farnesylation.

IT **197911-38-9P 197911-53-8P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of piperazine-2,5-dione derivs. as inhibitors of farnesyl-protein transferase)

L30 ANSWER 32 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:672280 HCAPLUS

DOCUMENT NUMBER: 127:346413

TITLE: Preparation of N-heterocyclylalkylpiperazinones as farnesyl protein transferase inhibitors

INVENTOR(S): Wei, Dong D.; Williams, Theresa M.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Wei, Dong D.; Williams, Theresa M.

SOURCE: PCT Int. Appl., 135 pp.

CODEN: PIXXD2

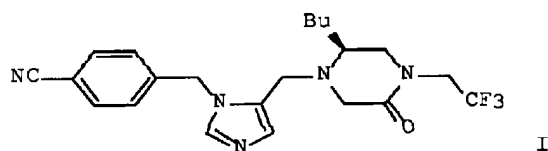
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9736593	A1	19971009	WO 1997-US5144	19970327 <--
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2249599	AA	19971009	CA 1997-2249599	19970327 <--
AU 9725548	A1	19971022	AU 1997-25548	19970327 <--
AU 706495	B2	19990617		
EP 921801	A1	19990616	EP 1997-917116	19970327 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2000507582	T2	20000620	JP 1997-535473	19970327 <--
PRIORITY APPLN. INFO.:			US 1996-14593P	P 19960403
			GB 1996-13460	A 19960627
			WO 1997-US5144	W 19970327
OTHER SOURCE(S):			MARPAT 127:346413	
GI				



AB R1A1[C(R1a)2]nA2[C(R1a)2]nZ[C(R1b)2]pZ1Z2R [I; A1,A2 = bond, CH:CH, CO, O, CONH, etc.; R = (un)substituted (cyclo)alkyl; R1 = H, (un)substituted heterocyclyl, -aryl, -alk(en)yl; R1a,R1b = H, alkyl, acyl, heterocyclyl, aryl, etc.; Z = bond or (un)substituted heterocyclyl; Z1 = CH2, CO, SOO-2; Z2 = (un)substituted (3-oxo)piperazine-1,4-diyl, -1,4-diazepine-1,4-diyl; n,p = 0-4] were prepd. Thus, (S)-BuCH(NHCO2CMe3)CH2NHCH2CF3 (prepn. given) was cyclocondensed with ClCH2COCl and the deprotected product N-alkylated with 1-(4-cyanobenzyl)imidazole-5-carboxaldehyde (prepn. given) to give, after acidification, I.2HCl. Data for biol. activity of I were given.

IT 198084-17-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of N-heterocyclylalkylpiperazinones as farnesyl protein transferase inhibitors)

L30 ANSWER 33 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:672278 HCAPLUS

DOCUMENT NUMBER: 127:331503

TITLE: Diazacyloalkanones as inhibitors of farnesyl-protein transferase

INVENTOR(S): Dinsmore, Christopher J.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Dinsmore, Christopher J.

SOURCE: PCT Int. Appl., 117 pp.

CODEN: PIXXD2

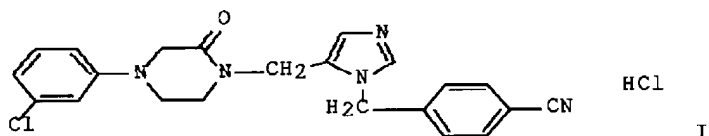
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9736591	A1	19971009	WO 1997-US4750	19970327 <--
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2250587	AA	19971009	CA 1997-2250587	19970327 <--
AU 9725879	A1	19971022	AU 1997-25879	19970327 <--
AU 707347	B2	19990708		
EP 900081	A1	19990310	EP 1997-917604	19970327 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2001518067	T2	20011009	JP 1997-535357	19970327 <--
PRIORITY APPLN. INFO.:				
			US 1996-14792P	P 19960403
			GB 1996-10338	A 19960517
			WO 1997-US4750	W 19970327
OTHER SOURCE(S): MARPAT 127:331503				
GI				



AB Diazacycloalkanones which inhibit farnesyl-protein transferase and the farnesylation of the oncogene protein Ras were prepd. Thus, 4-imidazolemethanol was tritylated, a acetylated, treated with 4-BrCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CN and deblocked to give 1-(4-cyanobenzyl)-5-hydroxymethylimidazole which was oxidized to the aldehyde and treated with 3-ClC<sub>6</sub>H<sub>4</sub>N(CH<sub>2</sub>CO<sub>2</sub>Me)CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>.HCl to give the piperazinone I. I had an IC<sub>50</sub> for inhibition of human FPTase of .1toeq.10 .mu.M.

IT **197853-30-8P 197853-33-1P**  
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of diazacycloalkanones as inhibitors of farnesyl-protein transferase)

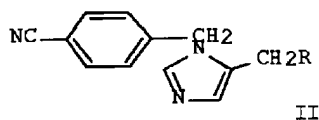
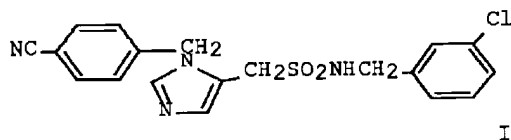
L30 ANSWER 34 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1997:672270 HCAPLUS  
 DOCUMENT NUMBER: 127:318953  
 TITLE: Preparation of imidazole derivatives as inhibitors of farnesyl-protein transferase  
 INVENTOR(S): Bergman, Jeffrey; Dinsmore, Christopher  
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Bergman, Jeffrey; Dinsmore, Christopher  
 SOURCE: PCT Int. Appl., 61 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9736583	A1	19971009	WO 1997-US5170	19970331 <--
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU,				

IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX,  
NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN,  
YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB,  
GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN,  
ML, MR, NE, SN, TD, TG

CA 2250143 AA 19971009 CA 1997-2250143 19970331 <--  
AU 9725968 A1 19971022 AU 1997-25968 19970331 <--  
AU 715604 B2 20000203  
EP 959883 A1 19991201 EP 1997-917711 19970331 <--  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI  
JP 2000507584 T2 20000620 JP 1997-535483 19970331 <--  
US 1996-14668P P 19960403  
GB 1996-10654 A 19960521  
WO 1997-US5170 W 19970331

GI



AB The present invention describes compds. (R6)rVA1(CR1a2)nA2(CR1b2)n(WR7)t(CR22)pA3(CR22)pXR3R4 [R1a, R1b, R2 = H, aryl, heterocycle, cycloalkyl, alkenyl, alkynyl, R8O, R9S(O)m, (R8)2NCO, R8CONR8, CN, NO2, (R8)2NC(NR8), R8CO, R8O2C, N3, N(R8)2, R9O2CNR8, (un)substituted alkyl; R3, R4 = H, F, Cl, Br, N(R8)2, CF3, NO2, R8O, R9S(O)m, (R8)2NCO, R8CONH, H2NC(NH), R8CO, R8O2C, N3, CN, R9O2CNR8, alkyl, (un)substituted aryl, (un)substituted heterocyclyl; A3 = NR5S(O)m, S(O)mNR5; m = 0 - 2; R5 = H, (un)substituted aryl, (un)substituted heterocyclyl, (un)substituted cycloalkyl, (un)substituted alkyl; R6, R7 = H, aryl, heterocyclyl, cycloalkyl, alkenyl, alkynyl, perfluoroalkyl, F, Cl, Br, R8O, R9S(O)m, R8CONR8, CN, NO2, (R8)2NC(NR8), R8CO, R8O2C, N3, N(R8)2, R9O2CNR8, (un)substituted alkyl; R8 = H, alkyl, aryl, aralkyl; R9 = alkyl, aryl; A1, A2 = CH:CH, C.tplbond.C, CO, CONR8, NR8CO, O, NR8, SO2NR8, NR8SO2, S(O)m; A1A2 = bond; X = aryl, heteroaryl; V = H, heterocyclyl, aryl, alkyl, heteroalkyl, alkenyl, provided that V is not H if A1 = S(O)m and V is not H if A1 = bond, n = 0, and A2 = S(O)m; W = heterocyclyl; n, p = 0 - 4; r = 0 - 5, with r = 0 when V = H; t = 0, 1] which inhibit farnesyl-protein transferase (FPTase) and the farnesylation of the oncogene protein Ras and to chemotherapeutic compns.. Sulfonamide I.HCl was prepd. from imidazole II (R = OH) via amidation of sulfinyl chloride II (R = SOCl) with 3-ClC6H4CH2NH2 followed by S-oxidn. of sulfonamide II (R = SONHCH2C6H4Cl-3). I.HCl was tested in vitro with Ras peptides, bovine and human FPTase and in vivo with a v-ras line derived from Rat1 or NIH3T3 cells (no data).

IT 197786-21-3P 197786-28-0P 197786-35-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of imidazole derivs. as inhibitors of farnesyl-protein transferase and as antitumor agents)

IT 197786-45-1P, 3-(4-Cyanobenzyl)-4-[(methylamino)methyl]pyridine

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. of imidazole derivs. as inhibitors of farnesyl-protein  
transferase and as antitumor agents)

L30 ANSWER 35 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:641305 HCAPLUS

DOCUMENT NUMBER: 125:275663

TITLE: Preparation of 9-(piperidinoalkyl)fluorene-9-  
carboxamides and analogs as microsomal triglyceride  
transfer protein inhibitors

INVENTOR(S): Wetterau, John R. II; Sharp, Daru Young; Gregg,  
Richard E.; Biller, Scott A.; Dickson, John A.;  
Lawrence, R. Michael; Magnin, David R.; Poss, Michael  
A.; Robl, Jeffrey A.; et al.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 427 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

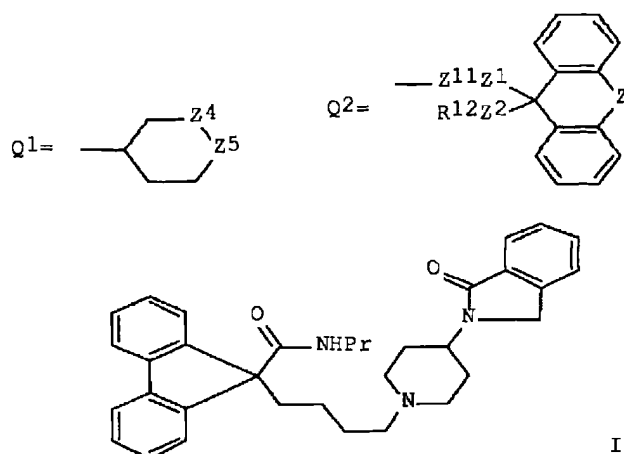
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9626205	A1	19960829	WO 1996-US824	19960201 <--
W: AU, BG, CA, CN, CZ, EE, FI, GE, HU, JP, KR, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SK, UA				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2091102	AA	19930907	CA 1993-2091102	19930305 <--
HU 67962	A2	19950529	HU 1993-627	19930305 <--
HU 218419	B	20000828		
JP 06038761	A2	19940215	JP 1993-46499	19930308 <--
EP 584446	A2	19940302	EP 1993-103697	19930308 <--
EP 584446	A3	19950426		
EP 584446	B1	20020619		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
AT 219514	E	20020715	AT 1993-103697	19930308 <--
PT 584446	T	20020930	PT 1993-103697	19930308
ES 2178640	T3	20030101	ES 1993-103697	19930308
AU 670930	B2	19960808	AU 1993-34064	19930309 <--
AU 9334064	A1	19930909		
US 5739135	A	19980414	US 1995-472067	19950606 <--
AU 9647631	A1	19960911	AU 1996-47631	19960201 <--
AU 699865	B2	19981217		
EP 886637	A1	19981230	EP 1996-903604	19960201 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
JP 11500442	T2	19990112	JP 1996-525679	19960201 <--
NZ 302055	A	20000228	NZ 1996-302055	19960201 <--
PL 185443	B1	20030530	PL 1996-322003	19960201
ZA 9601340	A	19970911	ZA 1996-1340	19960220 <--
FI 9703416	A	19970820	FI 1997-3416	19970820 <--
NO 9703821	A	19970820	NO 1997-3821	19970820 <--
LT 4367	B	19980825	LT 1997-152	19970919 <--

PRIORITY APPLN. INFO.:

US 1995-391901	A	19950221
US 1995-472067	A	19950606
US 1992-847503	A	19920306
US 1993-117362	A2	19930903
US 1994-284808	B2	19940805
WO 1996-US824	W	19960201

OTHER SOURCE(S): MAREPAT 125:275663

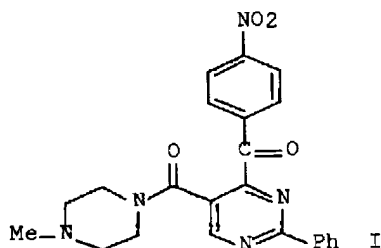
GI



AB R5Z3NRR6 [R = piperidyl group Q1; R5 = alkyl, alkoxy, (hetero)aryl, etc.; R6 = H, alk(en)yl; R5R6 = atoms to form a benzanellated ring; Z3 = CO or SO2; 1 of Z4, Z5 = NR1 and the other = CH2; R1 = e.g., (un)substituted aryl group Q2; R12 = H, (halo)alkyl, heteroaryl, etc.; Z = bond, O, S, alkylimino, etc.; Z1, Z2 = bond, O, SOO-2, CO, etc.; Z11 = bond, alkylene, arylene, etc.] were prepd. as microsomal triglyceride transfer protein inhibitors (no data). Thus, N-propyl-9-fluorene-carboxamide (prepn. given) was alkylated by I(CH2)4OSiMe2CMe3 (prepn. given) and the deprotected and iodinated product aminated by 2-(4-piperidinyl)-2,3-dihydro-1H-indol-1-one (prepn. given) to give title compd. I.

IT **182432-31-1P 182436-32-4P 182437-80-5P**  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of 9-(piperidinoalkyl)fluorene-9-carboxamides and analogs as microsomal triglyceride transfer protein inhibitors)

L30 ANSWER 36 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1995:75794 HCAPLUS  
DOCUMENT NUMBER: 122:55996  
TITLE: Studies of cerebral protective agents. VI. Synthesis of novel 4-(4-nitrobenzoyl)pyrimidine and related compounds with antianoxic activity  
AUTHOR(S): Ohkubo, Mitsuru; Kuno, Atsushi; Sakai, Hiroyoshi; Sugiyama, Yoshie; Takasugi, Hisashi  
CORPORATE SOURCE: New Drug Res. Lab., Fujisawa Pharmaceutical Co., Ltd., Osaka, 532, Japan  
SOURCE: Chemical & Pharmaceutical Bulletin (1994), 42(6), 1279-85  
CODEN: CPBTAL; ISSN: 0009-2363  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Novel pyrimidine derivs., possessing linkages between the aryl group and the pyrimidine nucleus at the C-4 position, were prepd. and tested for antianoxic activity in mice. Among them, 5-(4-methylpiperazin-1-ylcarbonyl)-4-(4-nitrobenzoyl)-2-phenylpyrimidine (FR 76659) (I) possessed significant antianoxic activity (10-100 mg/kg, i.p.) with low acute toxicity (LD50 > 1000 mg/kg, i.p.). Structure-activity relationship in regard to antianoxic activity of this series of compds. were examd.

IT 116904-35-9P 116904-65-5P 116904-66-6P  
159970-99-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(prepn. of antianoxic cerebral protective agent  
[(pyrimidinyl)carbonyl]piperazine)

L30 ANSWER 37 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:152980 HCAPLUS

DOCUMENT NUMBER: 120:152980

TITLE: Pyridobenzoxazepine and Pyridobenzothiazepine  
Derivatives as Potential Central Nervous System  
Agents: Synthesis and Neurochemical Study

AUTHOR(S): Liegeois, Jean Francois F.; Rogister, Francoise A.;  
Bruhwyler, Jacques; Damas, Jacques; Nguyen, Thuy  
Phuong; Inarejos, Maria Olvido; Chleide, Eric M. G.;  
Mercier, Michel G. A.; Delarge, Jacques E.

CORPORATE SOURCE: Laboratory of Medicinal Chemistry, University of  
Liege, Liege, B-4000, Belg.

SOURCE: Journal of Medicinal Chemistry (1994),  
37(4), 519-25

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

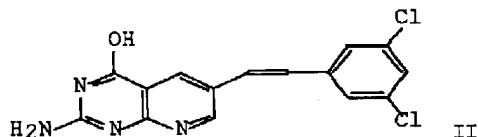
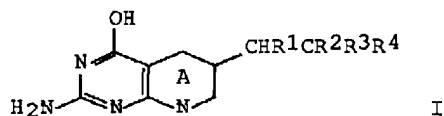
AB In order to characterize the pharmacol. profile of the different chem. classes of pyridobenzazepine derivs., a series of N-methylpiperazinopyrido[1,4]- and -[1,5]- benzoxa- and benzothiazepine derivs. were prepd. The affinities for D2, D1, 5-HT2, and cholinergic (M) receptors were measured. In comparison to dibenzazepine ref. compds., a strong decrease of the affinities was obsd., less pronounced, however, for the substituted analogs. Oxazepine and thiazepine analogs like clozapine (except 8-chloro-6-(4-methylpiperazin-1-yl)pyrido[2,3-b][1,4]benzoxazepine and 8-chloro-6-(4-methylpiperazin-1-yl)pyrido[2,3-b][1,4]benzothiazepine) were found to be inactive against apomorphine stereotypes. In the open-field test in rats, different mols. showed a high disinhibitory activity as obsd. with anxiolytic drugs. Moreover, 8-chloro-5-(4-methylpiperazin-1-yl)pyrido[2,3-b][1,5]benzoxazepine presented a clozapine-like profile that was confirmed in the behavioral model in dogs and showed most of the behavioral characteristics described for antipsychotic drugs. Its neurochem. profile, in particular the 5-HT2/D2 ratio, was also compatible with atypical antipsychotic activity.

IT 153143-99-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and cyclization of)

L30 ANSWER 38 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1993:147572 HCAPLUS  
DOCUMENT NUMBER: 118:147572  
TITLE: Preparation of pyridopyrimidine derivatives as  
antineoplastic agents  
INVENTOR(S): Gossett, Lynn Stacy; Shih, Chuan  
PATENT ASSIGNEE(S): Eli Lilly and Co., USA  
SOURCE: Eur. Pat. Appl., 16 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 511792	A2	19921104	EP 1992-303715	19920424 <--
EP 511792	A3	19921216		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, PT, SE				
US 5223503	A	19930629	US 1992-832243	19920207 <--
CA 2066898	AA	19921030	CA 1992-2066898	19920423 <--
JP 05117273	A2	19930514	JP 1992-109565	19920428 <--
PRIORITY APPLN. INFO.:			US 1991-692845	19910429
OTHER SOURCE(S):			MARPAT 118:147572	
GI				



AB Title compds. [I; ring A is pyrido or tetrahydropyrido; when A is pyrido, then R1R2 = bond, when A = tetrahydropyrido, R1,R2 = H; R3 = H, alkyl; R4 = (substituted) Ph, biphenyl, thienyl, pyridyl, naphthyl], were prepd. Thus, 2,4-diamino-6-[2-(3,5-dichlorophenyl)ethenyl]pyrido[2,3-d]pyrimidine was refluxed with aq. NaOH/dioxane to give title compd. II. The latter inhibited CCRF-CEM leukemia with IC50 = 6.4 mg/mL. An oral suspension was prepd contg. II.

IT **145769-31-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for neoplasm inhibitor)

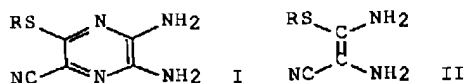
IT **95693-77-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for pyridopyrimidine neoplasm inhibitor)

L30 ANSWER 39 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1992:571474 HCAPLUS

DOCUMENT NUMBER: 117:171474  
TITLE: Cyanopyrazine derivatives and their manufacture  
INVENTOR(S): Kojima, Takakazu  
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04112877	A2	19920414	JP 1990-232592	19900904 <--
PRIORITY APPLN. INFO.:			JP 1990-232592	19900904
OTHER SOURCE(S):		CASREACT 117:171474; MARPAT 117:171474		
GI				



AB Title derivs. I [R = alkyl, aralkyl, cycloalkyl, alkenyl, (substituted aryl)] are manufd. by dimerizing II in the presence of an oxidn. catalyst. Thus, dimerization of II (R = Ph) in 1,2-dimethoxyethane/H2O in the presence of E.C. 1.11.1.7 and H2O2 under ice cooling for 5 h gave 54% I (R = Ph).

IT 143469-44-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, by dimerization of diamino(chlorophenylthio)acrylonitrile)

IT 143469-45-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, by dimerization of diamino(tolylthio)acrylonitrile)

L30 ANSWER 40 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:426413 HCAPLUS

DOCUMENT NUMBER: 117:26413

TITLE: Studies with polyfunctionally substituted heterocycles: synthesis of new pyridines, naphtho[1,2-b]pyrans, pyrazolo[3,4-b]pyridines and pyrazolo[1,5-a]pyrimidines

AUTHOR(S): Elnagdi, Mohamed Hilmy; Elghandour, Ahmed Hafiz  
Husein; Ibrahim, Mohamed Kamal Ahmed; Hafiz, Ibrahim  
Saad Abdel

CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt

SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences  
(1992), 47(4), 572-8

CODEN: ZNBSEN; ISSN: 0932-0776

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A variety of new polyfunctionally substituted pyridines, naphthopyrans and pyrazolopyrimidines were prepd. via reaction of ylidenemalononitriles with thiophenol, thionaphthol, naphthols and aminopyrazoles.

IT 141987-66-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and spectra of)

L30 ANSWER 41 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

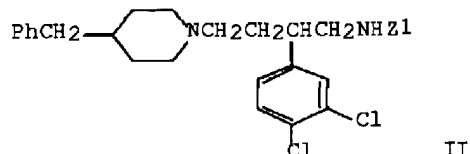
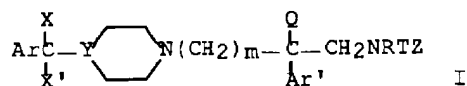
ACCESSION NUMBER: 1991:679818 HCAPLUS

DOCUMENT NUMBER: 115:279818

TITLE: Preparation of piperidine derivatives as neurokinin  
and substance P antagonists  
INVENTOR(S): Emonds-Alt, Xavier; Goulaouic, Pierre; Proietto,  
Vincenzo; Van Broeck, Didier  
PATENT ASSIGNEE(S): SANOFI, Fr.  
SOURCE: Eur. Pat. Appl., 84 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: French  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 428434	A2	19910522	EP 1990-403125	19901106 <--
EP 428434	A3	19911009		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FR 2654100	A1	19910510	FR 1989-14517	19891106 <--
FR 2654100	B1	19920221		
FR 2663329	A1	19911220	FR 1990-7534	19900615 <--
FR 2663329	B1	19921016		
FI 97540	B	19960930	FI 1990-5444	19901102 <--
FI 97540	C	19970110		
CA 2029275	AA	19910507	CA 1990-2029275	19901105 <--
NO 9004802	A	19910507	NO 1990-4802	19901105 <--
NO 177299	B	19950515		
NO 177299	C	19950823		
AU 9065838	A1	19910523	AU 1990-65838	19901105 <--
AU 649973	B2	19940609		
HU 56543	A2	19910930	HU 1990-7027	19901105 <--
US 5317020	A	19940531	US 1990-610093	19901105 <--
IL 111292	A1	19960331	IL 1990-111292	19901105 <--
RU 2084453	C1	19970720	RU 1990-4831627	19901105 <--
RU 2114828	C1	19980710	RU 1993-45020	19901105 <--
ZA 9008881	A	19910828	ZA 1990-8881	19901106 <--
JP 03206086	A2	19910909	JP 1990-300929	19901106 <--
PL 165758	B1	19950228	PL 1990-293823	19901106 <--
PL 165854	B1	19950228	PL 1990-293824	19901106 <--
PL 166565	B1	19950630	PL 1990-287644	19901106 <--
PL 166582	B1	19950630	PL 1990-303827	19901106 <--
IL 96241	A1	19960331	IL 1990-96241	19901115 <--
LV 10713	B	19951020	LV 1993-142	19930225 <--
US 5686609	A	19971111	US 1994-208672	19940311 <--
AU 9459245	A1	19940602	AU 1994-59245	19940331 <--
AU 668018	B2	19960418		
NO 9500239	A	19910507	NO 1995-239	19950123 <--
NO 180193	B	19961125		
NO 180193	C	19970305		
NO 9500240	A	19910507	NO 1995-240	19950123 <--
NO 179580	B	19960729		
NO 179580	C	19961106		
US 5618938	A	19970408	US 1995-479634	19950607 <--
FI 9502956	A	19950615	FI 1995-2956	19950615 <--
FI 9502957	A	19950615	FI 1995-2957	19950615 <--
FI 9800227	A	19980202	FI 1998-227	19980202 <--
PRIORITY APPLN. INFO.:				
			FR 1989-14517	A 19891106
			FR 1990-7534	A 19900615
			FI 1990-5444	A 19901102
			NO 1990-4802	A 19901105
			US 1990-610093	A3 19901105
			IL 1990-96241	A3 19901115
			US 1994-208672	A3 19940311
			FI 1995-2956	A 19950615

OTHER SOURCE(S): MARPAT 115:279818  
GI



AB The title compds. I [ $m = 1-3$ ; Ar, Ar' = thienyl, (substituted) Ph, etc.; X = H; X' = H, OH; or XX' = oxo, dialkylaminoalkoxyimino, etc.; Y = N, CX''; X'' = H or X'X'' = carbon-carbon bond; Q = H, alkyl, (CH<sub>2</sub>)<sub>q</sub>Am'; q = 2 or 3; Am' = piperidino, 4-benzylpiperidino, etc.; R = H, Me, (CH<sub>2</sub>)<sub>n</sub>L; n = 2-6; L = H, amino; T = CO, C(W)NH; W = O, S; Z = H, M, or OM when T = CO; or Z = M when T = C(W)NH; M = H, alkyl, (substituted) phenylalkyl, etc.] were prepd. I are neurokinin and substance P antagonists (no data). Reaction of amine II (Z1 = H) with 2,4-dichlorobenzoyl chloride in the presence of Et<sub>3</sub>N gave II (Z1 = 2,4-dichlorobenzoyl) isolated as its HCl salt. I are also useful as allergy and inflammation inhibitors (no data).

IT **135956-47-7P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of, as neurokinin antagonist)

L30 ANSWER 42 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:506008 HCAPLUS

DOCUMENT NUMBER: 115:106008

TITLE: Preparation of 3-aminomethylquinolines as antiarrhythmic drugs

INVENTOR(S): Cziaky, Zoltan; Korodi, Ferenc; Bilkei-Gorzo, Andras; Peszle, Judit; Frank, Laszlo; Balogh Korik, Pirooska; Fabian, Istvan, Mrs.

PATENT ASSIGNEE(S): Alkaloida Vegyeszeti Gyar, Hung.

SOURCE: Hung. Teljes, 18 pp.

CODEN: HUXXB

DOCUMENT TYPE: Patent

LANGUAGE: Hungarian

FAMILY ACC. NUM. COUNT: 1

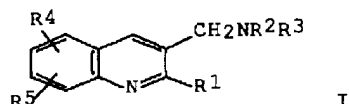
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
HU 54348	A2	19910228	HU 1989-1725	19890411 <--
HU 207048	B	19930301		

PRIORITY APPLN. INFO.: HU 1989-1725 19890411

OTHER SOURCE(S): MARPAT 115:106008

GI



AB The 3-aminomethylquinoline derivs. I (R1 = Cl, OH, alkoxy, aryloxy, heterocyclyl, etc.; R2, R3 = H, Ph, alkyl, etc.; R2R3 = alkylene; R4, R5 = H, halo, alkyl, alkoxy) are prepd. as antiarrhythmics. A mixt. of 4.24 g 2-chloro-3-chloromethylquinoline, 2.9 g 1-hydroxyethylpiperazine, 10 mL CHCl3 and 10 mL EtOH was stirred at 60.degree. for 6 h, followed by the addn. of 20 mL 2N HCl in EtOH, to give 2-chloro-3-[4-(2-hydroxyethyl)piperazine-1-yl]methyl quinoline-2HCl (II). II (10 mg/L) increased the elec. stimulation threshold and effective refractory period, and decreased the contractility of the isolated rabbit heart left atrium.

IT **135629-48-0P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and redn. of)

IT **135629-60-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as antiarrhythmic drug)

L30 ANSWER 43 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:492864 HCAPLUS

DOCUMENT NUMBER: 115:92864

TITLE: Synthesis and biological evaluation of  
2-desamino-2-methyl-5,10-dideazatetrahydrofolate

AUTHOR(S): Patil, Sharadbala D.; Kisliuk, R. L.; Gaumont, Y.;  
Nair, M. G.

CORPORATE SOURCE: Cancer Cent., Univ. South Alabama, Mobile, AL, 36688,  
USA

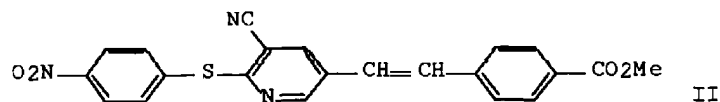
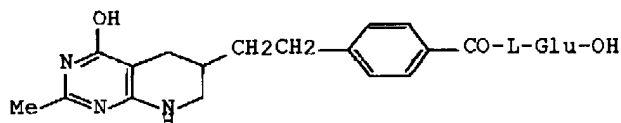
SOURCE: Chem. Biol. Pteridines, 1989 Proc. Int. Symp.  
Pteridines Folic Acid Deriv., 9th (1990),  
Meeting Date 1989, 1043-7. Editor(s): Curtius,  
Hans-Christoph; Ghisla, Sandro; Blau, Nenad. de  
Gruyter: Berlin, Fed. Rep. Ger.

CODEN: 57FTAQ

DOCUMENT TYPE: Conference

LANGUAGE: English

GI

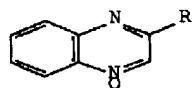


AB A report from a symposium on the prepn. of the title analog (I) of the antitumor agent 5,10-dideazatetrahydrofolate starting from styrylpyridine II. II was a relatively poor inhibitor of GAR-formyltransferase and exhibited only moderate inhibition of Manca human lymphoma cells in culture.

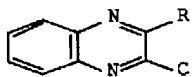
IT **135439-27-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and conversion of, to desamino(methyl)dideazatetrahydrofolate)

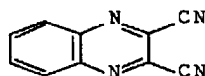
L30 ANSWER 44 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1990:478340 HCAPLUS  
DOCUMENT NUMBER: 113:78340  
TITLE: Quinoxalines. XXVII. The cyanation of 2-substituted quinoxaline 4-oxides with trimethylsilyl cyanide  
AUTHOR(S): Iijima, Chihoko; Miyashita, Akira  
CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan  
SOURCE: Chemical & Pharmaceutical Bulletin (1990), 38(3), 661-3  
CODEN: CPBTAL; ISSN: 0009-2363  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 113:78340  
GI



I



II



III

AB The deoxycyanation of 2-substituted quinoxaline 4-oxides I (R = Ph, MeO, EtO, Me<sub>2</sub>CH, Me<sub>3</sub>C, Et, Me, EtO<sub>2</sub>C, cyano, Cl, 4-MeC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>, etc.) with Me<sub>3</sub>SiCN in the presence of 1,8-diazabicyclo[5.4.0]undec-7-ene gave the corresponding 3-substituted 2-quinoxalinecarbonitriles II. However, in the case of I (R = 4-MeC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>) the substitution with cyanide ion proceeded together with deoxycyanation to give 2,3-quinoxalinedicarbonitrile (III).

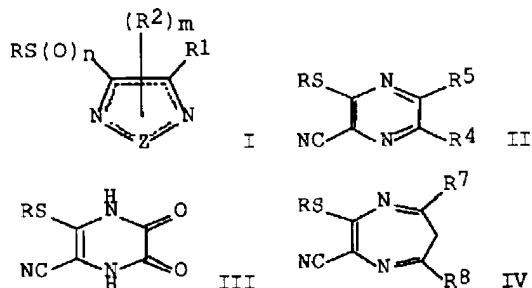
IT **128478-59-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

L30 ANSWER 45 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1990:459240 HCAPLUS  
DOCUMENT NUMBER: 113:59240  
TITLE: Preparation of pyrazine and 1,4-diazepine derivatives  
INVENTOR(S): Yagihara, Tomio; Matsui, Nobuo; Hamamoto, Isami; Hatano, Hiromi; Tazaki, Seiji  
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02049775	A2	19900220	JP 1988-233628	19880920 <--
PRIORITY APPLN. INFO.:			JP 1988-120729	19880519
OTHER SOURCE(S):	MARPAT	113:59240		

GI



AB The title compds. [I, more specifically II, III, and IV; R = (heterocycllyl)alkyl, aralkyl, cycloalkyl, alkenyl, (un)substituted aryl; n = 0, 1, 2; R1 = H, cyano, CONH2, (un)substituted CO2H; R2 = (alkyl)aryl, alkoxy carbonyl, oxo; m = 0, 1, 2; or R2R2 completing a ring; Z = CC or CCC; R4, R5 = H, alkyl, aralkyl, aryl, alkoxy carbonyl; or R4R5 completing a ring; R7, R8 = alkyl, aryl; or R7R8 completing a ring], useful as intermediates for pharmaceuticals, agrochems., perfumes, dyes, or polymers, are prepd. by cyclocondensation of (1) RSC(NH2):C(NH2)CN (V) with R4COCOR5 to II, (2) V with R6COCOR6 (R6 = Cl, imidazolyl) to III, and (3) V with R7COCH2COR8 to IV. Thus, benzil was added to a soln. of V in EtOH. After stirring 2 h at room temp., pptd. crystals were removed by filtration and recrystd. from benzene-n-hexane to give 70% II (R = Ph, R4 = R5 = Ph). Addnl. 42 I were prepd.

IT 128169-37-9P 128169-38-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, by cyclocondensation of diaminoacrylonitrile and dioxo compd.)

L30 ANSWER 46 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:570451 HCAPLUS

DOCUMENT NUMBER: 109:170451

TITLE: Preparation of pyrimidine derivatives as drugs for treating disease and disorders of cerebral blood vessels

INVENTOR(S): Takatani, Takao; Takasugi, Hisashi; Kuno, Atsushi; Sugiyama, Yoshie; Sakai, Hiroyoshi; Okubo, Mitsuru

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 31 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

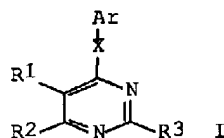
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63107966	A2	19880512	JP 1987-124326	19870520 <--
PRIORITY APPLN. INFO.:			JP 1986-117800	19860522
OTHER SOURCE(S):			CASREACT 109:170451; MARPAT 109:170451	

GI



AB The title compds. [I; Ar = (nitro or haloalkyl)aryl, fused benzene-heterocyclyl contg. N or O; X = bond, lower hydroxyalkylene, lower alkenylene, NH, S, CO; R1 = (esterified) CO2H, lower hydroxyalkyl, lower haloalkyl, (N-substituted) CONH2 or lower aminoalkyl; R2 = H, lower alkyl; optionally R1R2 completing (substituted) N-contg. heterocycle; R3 = aryl], were prep'd. as drugs e.g. for treating apoplexy. A mixt. of 6-bromomethyl-4-(3-nitrophenyl)-2-phenyl-5-pyrimidinecarboxylic acid Me ester and Me2NCH2CHNH2 in iso-PrOH was stirred at 70.degree. for 1 h to give 6-[2-(dimethylamino)ethyl]-4-(3-nitrophenyl)-5-oxo-2-phenyl-6,7-dihydropyrrolo[3,4-d]pyrimidine. The latter at 10 mg/kg i.p. extended the survival time of mice from 28.2 +/- 1.1 s (control) to 33.6 +/- 2.9 s when the mice were exposed to 100% N atm.

IT 116904-34-8P 116904-35-9P 116904-65-5P  
116904-66-6P 116904-78-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as drug for treating apoplexy)

L30 ANSWER 47 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:576424 HCAPLUS

DOCUMENT NUMBER: 107:176424

TITLE: Synthesis of 5,10-dideaza-5,6,7,8-tetrahydrofolic acid (DDATHF) and analogs

AUTHOR(S): Taylor, Edward C.; Wong, George S. K.; Fletcher, Stephen R.; Harrington, Peter J.; Beardsley, G. Peter; Shih, Chuan J.

CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA  
SOURCE: Chem. Biol. Pteridines, 1986, Pteridines Folic Acid

Deriv., Proc. Int. Symp. Pteridines Folic Acid Deriv.:

Chem., Biol. Clin. Aspects, 8th (1986),

61-4. Editor(s): Cooper, Bernard A.; Whitehead, V.

Michael. de Gruyter: Berlin, Fed. Rep. Ger.

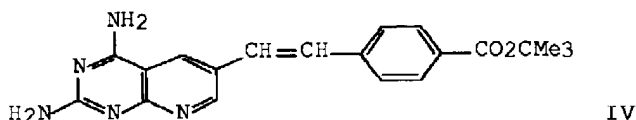
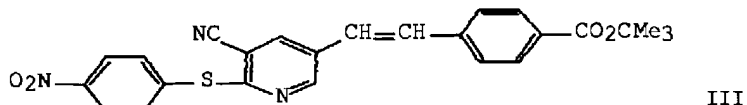
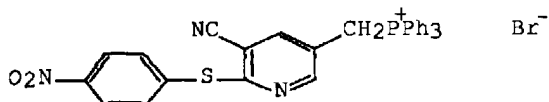
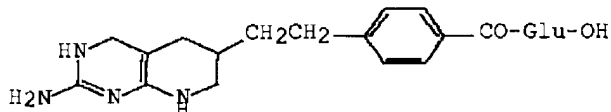
CODEN: 55HGAH

DOCUMENT TYPE: Conference

LANGUAGE: English

OTHER SOURCE(S): CASREACT 107:176424

GI



AB DDATHF (I) was prepd. in 14 steps from thiocyanacetamide and .beta.-ethoxymethacrolein. Two of the key steps were the Wittig reaction of phosphonium compd. II with tert-Bu p-formylbenzoate to give Wittig product III and the guanidine cyclization of III to give pyrido[2,3-d]pyrimidine IV. The glutamic acid moiety was introduced as di-Et glutamate. I was obtained as a mixt. of 2 diastereomers, which were sepd. via fractional crystn. of d-10-camphorsulfonic acid salts. The 10-Me analog of I was prepd. similarly. I and its analogs are potent inhibitors of cell growth in culture without significant effect on dihydrofolate reductase or thymidylate synthase.

IT 105580-38-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
(Wittig reaction of, with tert-Bu p-acetylbenzoate)

IT 105580-42-5P 105580-43-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

IT 95693-77-9P 95693-78-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for dideazatetrahydrofolic acid)

L30 ANSWER 48 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1987:33470 HCAPLUS

DOCUMENT NUMBER:

106:33470

TITLE:

N-[(Pyridopyrimidinylethyl)benzoyl]glutamic acid derivatives

INVENTOR(S):

Taylor, Edward C.; Beardsley, George Peter;  
Harrington, Peter J.; Fletcher, Stephen R.

PATENT ASSIGNEE(S):

Princeton University, USA

SOURCE:

PCT Int. Appl., 47 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8605181	A1	19860912	WO 1986-US368	19860224 <--
W:	AU, DK, HU, JP, KR, SU			
RW:	AT, BE, CH, DE, FR, GB, IT, LU, NL, SE			
ZA 8601235	A	19861029	ZA 1986-1235	19860219 <--

AU 8655108	A1	19860924	AU 1986-55108	19860224 <--
AU 578813	B2	19881103		
EP 215063	A1	19870325	EP 1986-901675	19860224 <--
EP 215063	B1	19931103		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
HU 41785	A2	19870528	HU 1986-2011	19860224 <--
HU 196202	B	19881028		
JP 62502535	T2	19871001	JP 1986-501296	19860224 <--
JP 08022860	B4	19960306		
AT 96790	E	19931115	AT 1986-901675	19860224 <--
US 4684653	A	19870804	US 1986-835457	19860303 <--
ES 552684	A1	19870316	ES 1986-552684	19860305 <--
IL 78059	A1	19890630	IL 1986-78059	19860306 <--
CA 1276637	A1	19901120	CA 1986-503509	19860307 <--
CN 86101475	A	19870121	CN 1986-101475	19860308 <--
CN 1016174	B	19920408		
DK 8604721	A	19861219	DK 1986-4721	19861002 <--
DK 168666	B1	19940516		
ES 557174	A1	19871216	ES 1986-557174	19861031 <--
SU 1676449	A3	19910907	SU 1986-4028461	19861103 <--
US 4845216	A	19890704	US 1987-74623	19870717 <--
US 4927828	A	19900522	US 1988-220944	19880628 <--
US 5026851	A	19910625	US 1989-341497	19890421 <--
CA 1308411	A2	19921006	CA 1990-615803	19900731 <--
JP 08193084	A2	19960730	JP 1995-228382	19950905 <--

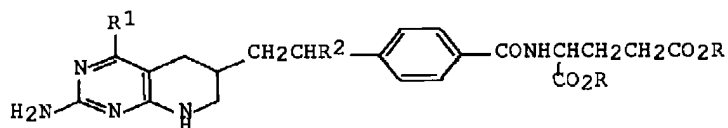
PRIORITY APPLN. INFO.:

US 1985-709622	19850308
EP 1986-901675	19860224
WO 1986-US368	19860224
US 1986-835457	19860303
CA 1986-503509	19860307
US 1986-871539	19860606
US 1987-74623	19870717

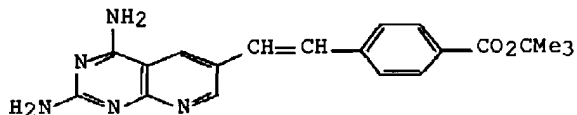
OTHER SOURCE(S):

CASREACT 106:33470

GI



I



II

AB N-[(Pyridopyrimidinylalkyl)benzoyl]-L-glutamic acids I (R = H; R1 = NH2, OH; R2 = H, Me, Et) and their 5,6,7,8-tetradehydro analogs were prepd. as neoplasm inhibitors. Thus, a triphenyl(3-pyridinylmethyl)phosphonium bromide deriv. underwent a Wittig reaction with 4-HCOC6H4CO2CMe3, followed by ammonolysis and cyclocondensation with guanidine to give [(pyridopyrimidinyl)ethenyl]benzoate II. The latter was converted in 6 steps to L-I (R = Et, R1 = OH, R2 = H), which was deesterified with CF3CO2H to give L-I (R = R2 = H, R1 = OH) (III). In mice 50 mg III/kg/day i.p. for 8 days gave 100% inhibition of, e.g., lymphosarcoma 6C3HED.

IT 87373-60-2

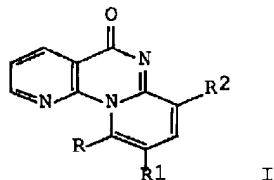
RL: RCT (Reactant); RACT (Reactant or reagent)  
(bromination of)

IT 95693-77-9P 105580-38-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)  
(prepn. and Wittig reaction of, with formylbenzoates and acetophenones)  
IT **88553-19-9P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and Wittig reaction of, with phosphines and formylbenzoate  
ester)  
IT **95674-62-7P 105580-39-0P 105580-40-3P**  
**105580-42-5P 105580-43-6P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and ammonolysis of)

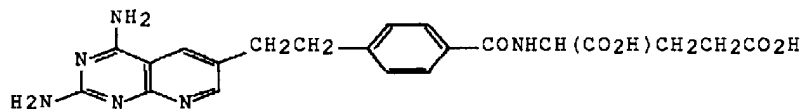
L30 ANSWER 49 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1985:504912 HCAPLUS  
DOCUMENT NUMBER: 103:104912  
TITLE: Synthesis and diuretic activity of  
pyrido[2,3-d]pyrimidones and related compounds  
AUTHOR(S): Monge, Antonio; Martinez-Merino, Victor;  
Cenarruzabeitia, Edurne; Lasheras, Berta;  
Fernandez-Alvarez, Eldiberto  
CORPORATE SOURCE: Dep. Quim. Org. Farmac., Spain  
SOURCE: European Journal of Medicinal Chemistry (1985  
, 20(1), 61-6  
CODEN: EJMCA5; ISSN: 0223-5234  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 103:104912  
GI



AB Dipyridopyrimidines I (R = H, 2-chloronicotinamido; R1 = H, Me; R2 = H, Me, 2-chloronicotinamido, NH2), which were prepd., showed diuretic activity. A mixt. of 2-chloronicotinoyl chloride and 2-aminopyridine in PhMe was heated to give I (R = R1 = R2 = H).  
IT **97936-26-0P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and cyclocondensation of)  
IT **97936-34-0P**  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. and diuretic activity of)  
IT **97936-25-9P 97936-27-1P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

L30 ANSWER 50 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1985:406676 HCAPLUS  
DOCUMENT NUMBER: 103:6676  
TITLE: Synthesis of the antileukemic agents  
5,10-dideazaaminopterin and 5,10-dideaza-5,6,7,8-

AUTHOR(S): tetrahydroaminopterin  
Taylor, Edward C.; Harrington, Peter J.; Fletcher,  
Stephen R.; Beardsley, G. Peter; Moran, Richard G.  
CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA  
SOURCE: Journal of Medicinal Chemistry (1985),  
28(7), 914-21  
CODEN: JMCMAR; ISSN: 0022-2623  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 103:6676  
GI



AB 5,10-Dideazaaminopterin (I) and 5,10-dideaza-5,6,7,8-tetrahydroaminopterin were prep'd. from pyridine precursors. These compds. exhibit significant in vivo activity against L1210 leukemia that is comparable to that obsd. with methotrexate.

IT 87373-60-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(bromination of)

IT 95674-62-7P 95693-78-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and amination of)

IT 95693-77-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and reaction of, with ethoxycarbonylbenzaldehyde)

IT 88553-19-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and reaction of, with triphenylphosphine)

L30 ANSWER 51 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1984:455505 HCAPLUS  
Correction of: 1984:103829  
DOCUMENT NUMBER: 101:55505  
Correction of: 100:103829  
TITLE: Synthesis and biological activity of L-5-deazafolic acid and L-deazaaminopterin: synthetic strategies to 5-deazapteridines  
AUTHOR(S): Taylor, Edward C.; Palmer, David C.; George, Thomas J.; Fletcher, Stephen R.; Tseng, Chi Ping; Harrington, Peter J.; Beardsley, G. Peter; Dumas, Donald J.; Rosowsky, Andre; Wick, Michael  
CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA  
SOURCE: Journal of Organic Chemistry (1983), 48(25), 4852-60  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB L-5-Deazafolic acid (I, R = R1 = H) was prepd. by the reductive amination of deazapterin II (R = Ac) with p-H2NC6H4CO-L-Glu(OMe)-OMe (III), followed by the sapon. of the resulting I (R = Ac, R1 = Me). L-5-Deazaaminopterin (IV) was prepd. similarly from 5-deazapteridine V and III. Pyrimidine VI was cyclized with HC(OMe)3 to give II (R = H), which was acetylated to give II (R = Ac). NCCH2CSNH2 was cyclized with EtOCH:CMcCO to give pyridinethione VII, which was converted to V in several steps in which the key was the cyclization of pyridine VIII with guanidine to give the di-Me acetal of V. 3-Formylthietane and its di-Me and ethylene acetals were prepd. as synthons for the pyridine ring of deazapteridines IX (R2 = R3 = H, R2R3 = bond). 2,4-Diamino-6-methyl-5-deazapteridine was prepd., but functionalization of the C-6 Me group was not possible. I is equipotent with methotrexate as an inhibitor of bovine liver dihydrofolate reductase and of L1210 murine leukemia cells.

IT 87373-63-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and acetalization of)

IT 87373-64-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and aminolysis of)

IT 87373-60-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and bromination of)

IT 87373-87-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and hydrolysis of)

IT 87373-62-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and reaction of, with nitrosodimethylaniline)

IT 87373-61-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and reaction of, with pyridine)

L30 ANSWER 52 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1984:103829 HCAPLUS

DOCUMENT NUMBER: 100:103829

TITLE: Synthesis and biological activity of L-5-deazafolic acid and L-deazaaminopterin: synthetic strategies to 5-deazapteridines

AUTHOR(S): Taylor, Edward C.; Palmer, David C.; George, Thomas J.; Fletcher, Stephen R.; Tseng, Chi Ping; Harrington, Peter J.; Beardsley, G. Peter

CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA

SOURCE: Journal of Organic Chemistry (1983), 48(25),

4852-60

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB L-5-Deazafolic acid (I, R = R1 = H) was prepd. by the reductive amination of deazapterin II (R = Ac) with p-H2NC6H4CO-L-Glu(OMe)-OMe (III), followed by the sapon. of the resulting I (R = Ac, R1 = Me). L-5-Deazaaminopterin (IV) was prepd. similarly from 5-deazapteridine V and III. Pyrimidine VI was cyclized with HC(OMe)3 to give II (R = H), which was acetylated to give II (R = Ac). NCCH2CSNH2 was cyclized with EtOCH:CMcCO to give pyridinethione VII, which was converted to V in several steps in which the key step was the cyclization of pyridine VIII with guanidine to give the di-Me acetal of V. 3-Formylthietane and its di-Me and ethylene acetals were prepd. as synthons for the pyridine ring of deazapteridines IX (R2 = R3 = H, R2R3 = bond). 2,4-Diamino-6-methyl-5-deazapteridine was prepd., but functionalization of the C-6 Me group was not possible. I is equipotent with methotrexate as an inhibitor of bovine liver dihydrofolate reductase and of L1210 murine leukemia cells.

IT 87373-63-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and acetalization of)

IT 87373-64-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and aminolysis of)

IT 87373-60-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and bromination of)

IT 87373-87-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and hydrolysis of)

IT 87373-62-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and reaction of, with nitrosodimethylaniline)

IT 87373-61-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and reaction of, with pyridine)

L30 ANSWER 53 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1984:68665 HCAPLUS

DOCUMENT NUMBER: 100:68665

TITLE: Synthesis and biological activity of 5-deazafolic acid and 5-deazaaminopterin

AUTHOR(S): Taylor, Edward C.; Tseng, Chi Ping; Harrington, Peter J.; Beardsley, G. Peter; Rosowsky, Andrew; Wick, Michael

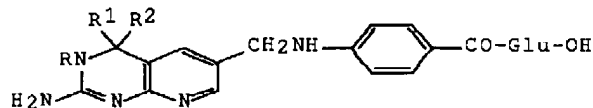
CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, USA

SOURCE: Chem. Biol. Pteridines, Proc. Int. Symp. Pteridines Folic Acid Deriv.: Chem., Biol. Clin. Aspects, 7th (1983), Meeting Date 1982, 115-19. Editor(s): Blair, John A. de Gruyter: Berlin, Fed. Rep. Ger. CODEN: 50NHAH

DOCUMENT TYPE: Conference

LANGUAGE: English

GI

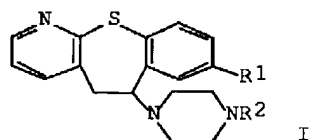


- AB Title compds. I (R = H, R1R2 = O; RR1 = bond, R2 = NH2) were prepd. by multistep procedures starting with the resp. cyclocondensation of 2,4-diamino-6(1H)-pyrimidinone with HC(CHO)3 and of NCCH2C(S)NH2 with EtOCH:CMcCHO. 5-Deazafolic acid is a potent inhibitor of dihydrofolate reductase. The cytotoxic activities of I were also examd.
- IT **87373-63-5P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and acetylation with methanol)
- IT **87373-64-6P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and aminolysis of)
- IT **87373-60-2P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and bromination of)
- IT **88553-20-2P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and elimination reaction of)
- IT **88553-19-9P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and reaction with pyridine)
- IT **87373-61-3P 88566-70-5P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

L30 ANSWER 54 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1976:421451 HCAPLUS  
DOCUMENT NUMBER: 85:21451  
TITLE: Psychotropic 6-piperazino-5,6-dihydrobenzo(b)pyrido(3,2-f)thiepins  
INVENTOR(S): Protiva, Miroslav; Bartl, Vaclav; Metysova, Jirina  
PATENT ASSIGNEE(S): Czech.  
SOURCE: Czech., 5 pp.  
CODEN: CZXXA9  
DOCUMENT TYPE: Patent  
LANGUAGE: Czech  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CS 159522	B	19750131	CS 1972-7366	19721101 <--
PRIORITY APPLN. INFO.:			CS 1972-7366	19721101

GI



AB The title compds. I [R1 = Cl or iso-Pr; R2 = H, Me, (CH2)3OH or CO2Et] were prepd. I had central nervous system depressant, cataleptic, and anticonvulsant activity (no data). Heating of 2-chloronicotinic acid (II) with 4-ClC6H4SH gave 2-(4-chlorophenylthio)nicotinic acid which was reduced with NaAl(OCH2CH2OMe)2H2 to 2-(4-chlorophenylthio)-3-pyridylcarbinol. Treatment with SOCl2 gave the HCl salt of 2-(4-chlorophenylthio)-3-chloromethylpyridine. The free base reacted with KCN in aq. EtOH giving 2-(4-chlorophenylthio)-3-pyridylacetonitrile which was hydrolyzed with KOH to 2-(4-chlorophenylthio)-3-pyridylacetic acid. Cyclization with polyphosphoric acid yielded 8-chlorobenzo[b]pyrido[3,2-f]thiepin-6(5H)-one. Redn. with NaBH4 gave the 6-hydroxy-5,6-dihydro analog which was transformed with SOCl2 to 6,8-dichloro-5,6-dihydrobenzo[b]pyrido[3,2-f]thiepin HCl. Substitution reactions with 1-methyl-, 1-(3-hydroxypropyl)- and 1-(ethoxycarbonyl)piperazine gave I [R1 = Cl, R2 = Me, (CH2)3OH, and CO2Et]. The latter was hydrolyzed with KOH to I (R1 = Cl, R2 = H). A similar synthesis starting from the reaction of II with 4-(iso-Pr)C6H4SH gave in nine steps I (R1 = iso-Pr, R2 = Me).

IT 51723-89-8P 51723-90-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and hydrolysis of)

L30 ANSWER 55 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1974:82882 HCAPLUS

DOCUMENT NUMBER: 80:82882

TITLE: Neurotropic and psychotropic agents. LXV. 8-Chloro and 8-isopropyl-6-piperazinobenzo[b]pyrido[3,2-f]thiepins

AUTHOR(S): Bartl, V.; Metysova, J.; Protiva, M.

CORPORATE SOURCE: Res. Inst. Pharm. Biochem., Prague, Czech.

SOURCE: Collection of Czechoslovak Chemical Communications (1973), 38(9), 2778-87

CODEN: CCCCAK; ISSN: 0010-0765

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The title compds., esp. I-IV, were prepd. as potential neuroleptics. Reaction of 2-chloronicotinic acid with 4-chloro- and 4-isopropylbenzenethiol gave 2-(4-chlorophenylthio)- and 2-(4-isopropylphenylthio)nicotinic acid which were converted in 4 steps to 2-(4-chlorophenylthio)- and 2-(4-isopropylphenylthio)-3-pyridineacetic acid. Cyclization with polyphosphoric acid yielded 8-chloro- (V) and 8-isopropylbenzo[b]pyrido[3,2-f]thiepin-6(5H)-one (VI). V and VI treated with 1-methylpiperazine (VII) and TiCl4 in C6H6 gave I and II. V and VI were reduced with NaBH4 and the alcs. obtained converted with SOCl2 to 6,8-dichloro-5,6-dihydrobenzo[b]pyrido[3,2-f]-thiepin (VIII) and 6-chloro-8-isopropyl-5,6-dihydrobenzo[b]-pyrido[3,2-f]thiepin (IX). VIII and IX treated with VII, 1-(3-hydroxypropyl)piperazine and 1-(ethoxycarbonyl)piperazine gave III, IV, and the corresponding analogs. 6-[4-(Ethoxycarbonyl)-1-piperazinyl]-8-chloro-5,6-dihydrobenzo[b]pyrido[3,2-f]thiepin was hydrolyzed to 6-1-piperazinyl-8-chloro-5,6-dihydrobenzo[b]-pyrido[3,2-f]thiepin.

IT 51723-89-8P 51723-90-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

L30 ANSWER 56 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1972:488314 HCAPLUS  
DOCUMENT NUMBER: 77:88314  
TITLE: Pesticidal 2-substituted-3-cyano-5-nitropyridines  
INVENTOR(S): Freeman, Peter F. H.  
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.  
SOURCE: U.S., 8 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3674877	A	19720704	US 1970-42858	19700602 <--
PRIORITY APPLN. INFO.:			US 1970-42858	19700602

GI For diagram(s), see printed CA Issue.

AB 5-Nitronicotinonitrile derivs. (I, R = Cl, OH, amino, arylamido, alkylthio, arylthio, arylidithio, aryloxy), 3-cyano-1-methyl-5-nitro-2-pyridone, and 2-chloro-3-cyano-1-ethyl-5-nitropyridinium fluoroborate were prepd. from the dihydropyridine derivs. (II, R1 = H, Me; X = O, S) obtained by condensation of NaC(NO2)(CHO)2 with NCCH2CXNH2. Thus, I (R = Cl) was prepd. by treating II (R1 = H, X = O) with PCl5 and POCl3. I (R = NHCH2CO2Et) was prepd. by treating I (R = Cl) with EtO2CCH2NH2.HCl and NaOAc. Many of the above 32 compds. were agricultural fungicides and insecticides. Thus, I (R = pyrrolidino) at 125 ppm killed Aphis fabae and Megoura vicia; I (R = Cl) at 500 ppm was more effective than Thiram against Pythium ultimum.

IT **31309-28-1P 31309-29-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

L30 ANSWER 57 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1972:126788 HCAPLUS  
DOCUMENT NUMBER: 76:126788  
TITLE: Antiedematous 2-(phenylthio)- and 2-phenoxyypyridines  
INVENTOR(S): Blum, Jean  
SOURCE: Fr. Demande, 12 pp.  
CODEN: FRXXBL  
DOCUMENT TYPE: Patent  
LANGUAGE: French  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2068429	A5	19710827	FR 1969-39113	19691114 <--
FR 2068429	B1	19730112		
PRIORITY APPLN. INFO.:			FR 1969-39113	19691114

GI For diagram(s), see printed CA Issue.

AB Re-fluxing nicotinamide 1-oxide with POCl3 gave I (R = Cl) (II). Refluxing II with aq. EtOH-PhOK gave I (R = PhO) (III). Similarly prepd. were I (R = PhS, 2,3-Me2C6H3S, m-F3CC6H4S). Refluxing III with aq. EtOH-KOH gave 2-phoxynicotinic acid (IV); other nitriles were similarly hydrolyzed. Heating I (R = PhS) with NaN3, LiCl, and NH4Cl in HCONMe2 at 130.degree. gave 2-(phenylthio)-3-(5-tetrazolyl)pyridine (V). At 100 mg/-kg, III gave 42% inhibition of carrageenan induced edema in rat paws.

IT **35620-70-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

L30 ANSWER 58 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1971:99891 HCAPLUS  
 DOCUMENT NUMBER: 74:99891  
 TITLE: Pesticidal 2-substituted 3-cyano-5-nitropyridines  
 INVENTOR(S): Barton, John E. D.; Freeman, Peter F. H.  
 PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.  
 SOURCE: Ger. Offen., 45 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2029079	A	19710121	DE 1970-2029079	19700612 <--
ZA 7003779	A	19720126	ZA 1970-3779	19700603 <--
NL 7008411	A	19701215	NL 1970-8411	19700610 <--
FR 2046711	A7	19710312	FR 1970-21497	19700611 <--
FR 2046711	B3	19730316		
ES 380702	A1	19720816	ES 1970-380702	19700612 <--
BR 7019726	A0	19730220	BR 1970-219726	19700612 <--
PRIORITY APPLN. INFO.:			GB 1969-29864	19690612

GI For diagram(s), see printed CA Issue.  
 AB Comps. of the new fungicidal (esp. active against fungi originating in the soil), in some cases insecticidal, nonherbicidal title compds. (I), II, and III for plants are reported. Thus, refluxing 3-cyano-5-nitro-2-pyridone in PCl5-POCl3 gave I (R = Cl) (IV). Refluxing IV, Et glycinate-HCl, and AcONa in aq. EtOH gave I (R = NHCH2CO2Et). Among 29 compds. similarly prepd. or described were I (R given): NH2, NHPH, NMe2, NHBz, SPr-iso, SCH2CH2CN, SCH2CO2Et, SCH2Ph, OC6H4Cl-p, II, and III.  
 IT **31309-28-1P 31309-29-2P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

L30 ANSWER 59 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1969:501819 HCAPLUS  
 DOCUMENT NUMBER: 71:101819  
 TITLE: Unusual leaving groups in cyclizations of the quinoxaline series. II  
 AUTHOR(S): Dahn, Hans; Nussbaum, Jeannine  
 CORPORATE SOURCE: Univ. Lausanne, Lausanne, Switz.  
 SOURCE: Helvetica Chimica Acta (1969), 52(6), 1661-71  
 CODEN: HCACAV; ISSN: 0018-019X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: French  
 OTHER SOURCE(S): CASREACT 71:101819

GI For diagram(s), see printed CA Issue.  
 AB 2,3-(RR1-Substituted)quinoxalines (I) (where R = H, OH, Cl, CN, CO2H, CONH2, CH2Ph, or Bz; and R1 = p-MeOC6H4 or Ph) were cyclized with HONH2 to give 3-(R1-substituted)isoxazolo [4,5-b]quinoxalines (II) and with PhNHNH2 to give 3-(R1-substituted)pyrazolo[4,5-b]quinoxalines (III). I (where R = Me or Ph) were not cyclized. The displacement of H in I (R = H) is explained in terms of the osazone formation theory.  
 IT **23773-91-3P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

L30 ANSWER 60 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1965:51669 HCAPLUS  
 DOCUMENT NUMBER: 62:51669

ORIGINAL REFERENCE NO.: 62:9138a-e  
TITLE: 4-Azathioxanthene derivatives  
INVENTOR(S): Jucker, E.; Ebnoether, A.  
PATENT ASSIGNEE(S): Sandoz Ltd.  
SOURCE: 11 pp.; Addn. to Belg. 611,216 (CA 58, 1461g).  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 638971		19640421	BE	<--
FR AD84820			FR	
FR M3323			FR	
NL 299465			NL	

PRIORITY APPLN. INFO.: CH 19621023

GI For diagram(s), see printed CA Issue.

AB The title compds. of general formula Ia are useful as antihistamines, serotonin antagonists, antiasthmatics, neuroleptics, or antidepressants. Thus, a mixt. of 78 g. 2-chloronicotinic acid and 145 g. p-chlorothiophenol was heated 3 hrs. at 170.degree. and cooled, the reaction product treated with 500 ml. ether and 1 l. satd. NaHCO<sub>3</sub> soln. to dissoln., the ether layer extd. with NaHCO<sub>3</sub> soln., and the combined aq. exts. adjusted to pH 5 with AcOH to ppt. 2-(p-chlorophenylthio)-3-carboxypyridine (I), m. 216-17.degree. (MeOH). A mixt. of 35 g. I and 350 g. polyphosphoric acid was heated at 150.degree. 1 hr. and at 180.degree. 2 hrs., cooled to about 100.degree., and drowned with good agitation in 1500 ml. H<sub>2</sub>O, the ppt. filtered off, agitated 10 min. with 200 ml. 10% caustic soda, filtered off again, washed well with H<sub>2</sub>O, and dried to give 7-chloro-4-azathioxanthone (II), m. 194-5.degree. (AcOH). Mg turnings (2.43 g.) activated with iodine were covered with 10 ml. tetrahydrofuran (THF), 0.3 ml. ethylene bromide was added to start the reaction, a soln. of 14.7 g. 1-methyl-4-chloropiperidine in 25 ml. abs. THF added dropwise at such a rate that the reaction mixt. stayed at a boil, the mixt. heated 1-2 hrs. until most of the Mg was in soln. and cooled, 12.4 g. II added portionwise at 20-5.degree., the mixt. agitated 20 min. at room temp., poured into 300 ml. 10% NH<sub>4</sub>Cl, and extd. with CH<sub>2</sub>Cl<sub>2</sub>, and the ext. dried over MgSO<sub>4</sub> and evapd. to give 4-aza-7-chloro-9-(1-methyl-4-piperidyl)thioxanthidrol (III), m. 225-6.degree. (Me<sub>2</sub>CO). A mixt. of 10 g. III, 25 ml. H<sub>2</sub>O, and 75 ml. H<sub>2</sub>SO<sub>4</sub> was heated 20 min. to 140.degree. and drowned in 500 ml. ice H<sub>2</sub>O, the soln. made alk. with 50% caustic soda and extd. with CH<sub>2</sub>Cl<sub>2</sub>, and the ext. dried over K<sub>2</sub>CO<sub>3</sub> and evapd. to give 4-aza-7-chloro-9-(1-methyl-4-piperidylidene)thioxanthene, m. 150-2.degree. (Me<sub>2</sub>CO). Similarly prepd. were the following 4-azathioxanthenes (substituents and m.p. given): 7-Br, 190-3.degree. (AcOH); 7-Me, 153-4.degree. (Me<sub>2</sub>CO); 3,7-MeCl, 235-6.degree. (AcOH). Also prepd. were 4-azathioxanthidrols (same data): 7-bromo-9-(1-methyl-4-piperidyl), 227-37.degree. (decompn.) (EtOH); 7-methyl-9-(1-methyl-4-piperidyl), 185-6.degree. (EtOH); 3-methyl-7-chloro-9-(1-methyl-4-piperidyl), 208-10.degree. (Me<sub>2</sub>CO); 7,9-Cl-[Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>], 175-7.degree. (EtOAc); 7,9-Me[Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>], 172-4.degree. (Me<sub>2</sub>CO). The following 4-azathioxanthenes were also prepd. (same data): 7-bromo-9-(1-methyl-4-piperidylidene), 166-8.degree. (Me<sub>2</sub>CO); 7-methyl-9-(1-methyl-4-piperidylidene), 130-2.degree. (hexane); 3-methyl-7-chloro-9-(1-methyl-4-piperidylidene), 155-6.degree. (Me<sub>2</sub>CO); 7,9-Cl(Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CH:), - [fumarate m. 179-81.degree. (decompn.) (MeOH)]; 7,9-Me(Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CH:), - [H fumarate m. 195-6.degree. (decompn.) (MeOH)]. The following IV (used as intermediates) were also prepd. (R, R<sub>1</sub>, R<sub>2</sub>, and m.p. given): BrCO<sub>2</sub>H, H, 220-1.degree. (MeOH); Me, CO<sub>2</sub>H, H, 217-18.degree. (EtOH); Cl, CN, Me, 135-6.degree. (Me<sub>2</sub>CO); Cl, CO<sub>2</sub>H, Me, 212-13.degree..

IT 955-63-5, Nicotinonitrile, 2-[(p-chlorophenyl)thio]-6-methyl-  
(prepn. of)

L30 ANSWER 61 OF 61 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1961:38071 HCAPLUS  
DOCUMENT NUMBER: 55:38071  
ORIGINAL REFERENCE NO.: 55:7425a-e  
TITLE: Reductions and 1,2,3-tricarbonyl compounds. XIX.  
.gamma.-Aryl-.alpha.,.beta.-dioxobutyramides  
AUTHOR(S): Dahn, H.; Rotzler, G.  
CORPORATE SOURCE: Univ. Basel, Switz.  
SOURCE: Helvetica Chimica Acta (1960), 43, 1555-61  
CODEN: HCACAV; ISSN: 0018-019X  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
OTHER SOURCE(S): CASREACT 55:38071  
GI For diagram(s), see printed CA Issue.  
AB cf. CA 54, 19635d. Refluxing I (obtained from aromatic or heterocyclic aldehydes with glyoxal and KCN; Dahn, et al., CA 49, 13209b) 1 hr. with 40% AcOH or 0.01N H2SO4 or heating I with H2O and Amberlite IR (H form) to 70.degree. gives RCH2COCOC(=O)NH2.H2O (II) and lactones (III). Oxidn. of II with 1 mole HIO4 gives the RCH2CO2H, NH3, and (COOH)2; condensation of II with o-phenylenediamine gives 3-substituted-quinoxaline-2-carboxamide, which can be hydrolyzed to the free acid and decarboxylated to 2-substituted-quinoxaline. Phenylhydrazine reacts with the middle CO group of II to form a phenylhydrazone, and with the oxo and amide groups to form a pyrazolone. The middle CO group is hydrated; in the presence of MeOH, a half acetal, RCH2COC(OMe)(OH)CONH2 is formed. The following II are prepd. (R given): Ph, m. 108-10.degree. (decompn.), .lambda. 295 m.mu. (all in EtOH); o-ClC6H4, .lambda. 305 m.mu.; p-MeOC6H4, m. 110-14.degree. (decompn.). 3-Arylquinoxaline-2-carboxamides prepd. were (aryl group given): PhCH2, m. 163.degree.; o-ClC6H4CH2, m. 193.degree.; p-MeOC6H4CH2, m. 165.degree.. 3-Benzylquinoxaline-2-carboxylic acid m. 145.degree. (decompn.); 2-benzylquinoxaline m. 38.5.degree., b.12 208-10.degree.; 2-(o-chlorobenzyl)quinoxaline m. 55.degree., b.0.01 114-16.degree.; 1-phenyl-3-benzyl-4-phenylazo-5-pyrazolone (IV) m. 153-4.degree.; the 3-(o-chlorobenzyl) analog of IV m. 166-9.degree.. Infrared spectral data are given.  
IT 101569-95-3, 2-Quinoxalinecarboxamide, 3-p-methoxybenzyl- (prepn. of)

=>  
=>

=> select hit rn 130 1-61  
E121 THROUGH E240 ASSIGNED

=> fil reg  
FILE 'REGISTRY' ENTERED AT 11:34:10 ON 19 MAY 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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STRUCTURE FILE UPDATES: 18 MAY 2004 HIGHEST RN 683203-75-0  
DICTIONARY FILE UPDATES: 18 MAY 2004 HIGHEST RN 683203-75-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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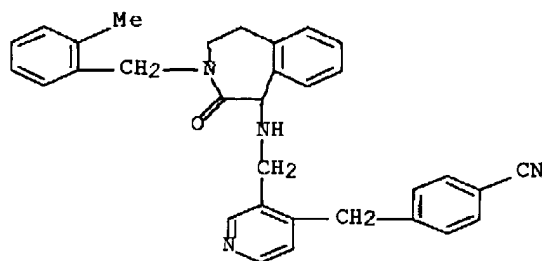
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=> d ide can 131 1-120

L31 ANSWER 1 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
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MF C32 H30 N4 O . 2 C4 H4 O4  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

CM 1

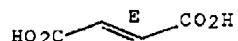
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CMF C32 H30 N4 O



CM 2

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CMF C4 H4 O4

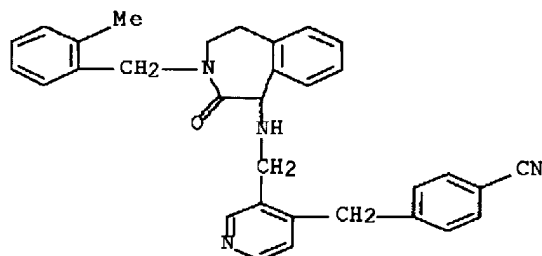
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:125099

L31 ANSWER 2 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 443927-03-5 REGISTRY  
CN Benzonitrile, 4-[[[3-[[[2,3,4,5-tetrahydro-3-[(2-methylphenyl)methyl]-2-oxo-1H-3-benzazepin-1-yl]amino]methyl]-4-pyridinyl]methyl]- (9CI) (CA INDEX NAME)  
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MF C32 H30 N4 O  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



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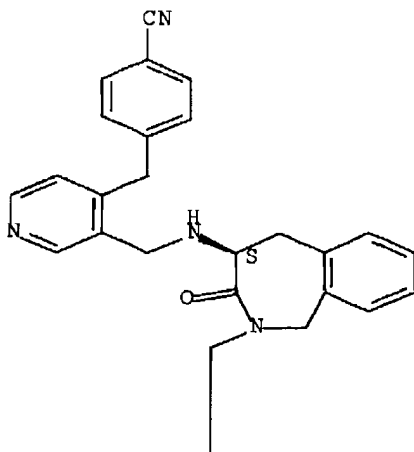
L31 ANSWER 3 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 443926-07-6 REGISTRY  
CN Benzonitrile, 4-[[[3-[[[(4S)-2,3,4,5-tetrahydro-2-[(2-methylphenyl)methyl]-3-oxo-1H-2-benzazepin-4-yl]amino]methyl]-4-pyridinyl]methyl]-, (2E)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)  
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MF C32 H30 N4 O . 2 C4 H4 O4  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

CM 1

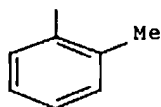
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CMF C32 H30 N4 O

Absolute stereochemistry.

PAGE 1-A



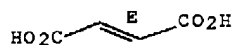
PAGE 2-A



CM 2

CRN 110-17-8  
CMF C4 H4 O4

Double bond geometry as shown.



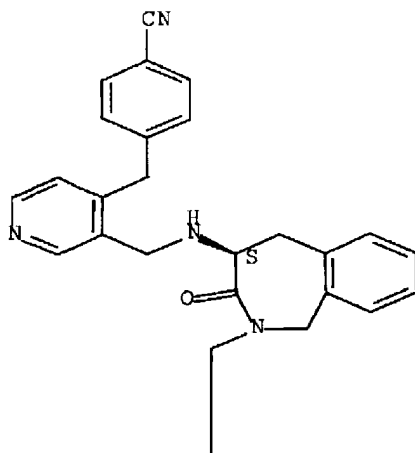
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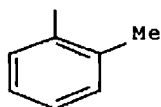
L31 ANSWER 4 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 443926-06-5 REGISTRY  
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FS STEREOSEARCH  
MF C32 H30 N4 O  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

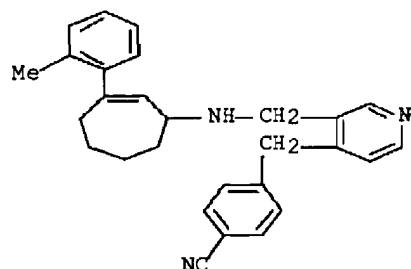
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:125098

L31 ANSWER 5 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **443304-56-1** REGISTRY  
CN Benzonitrile, 4-[[3-[[[3-(2-methylphenyl)-2-cyclohepten-1-yl]amino]methyl]-4-pyridinyl]methyl]-, (2E)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H29 N3 . 2 C4 H4 O4  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

CM 1

CRN 443304-55-0  
CMF C28 H29 N3



CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:109277

L31 ANSWER 6 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 443304-29-8 REGISTRY

CN Benzonitrile, 4-[[[3-[[[3-(phenylthio)phenyl]-2-cyclohepten-1-yl]amino]methyl]-4-pyridinyl]methyl]-, (2E)-2-butenedioate (1:2) (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C33 H31 N3 S . 2 C4 H4 O4

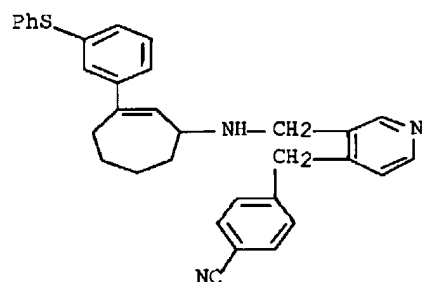
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

CM 1

CRN 443304-28-7

CMF C33 H31 N3 S



CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



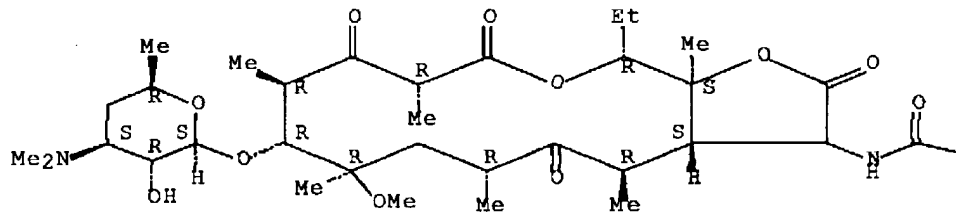
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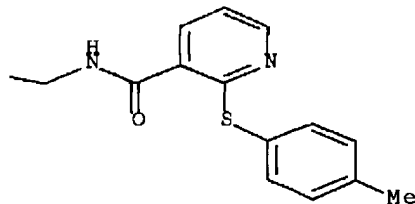
L31 ANSWER 7 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 439103-24-9 REGISTRY  
CN 3-Pyridinecarboxamide, N-[2-[[[(3aS,4R,6R,8R,9R,10R,12R,15R,15aS)-15-ethyltetradecahydro-8-methoxy-4,6,8,10,12,15a-hexamethyl-2,5,11,13-tetraoxo-9-[[[3,4,6-trideoxy-3-(dimethylamino)-.beta.-D-xylo-hexopyranosyl]oxy]-2H-furo[2,3-c]oxacyclotetradecin-3-yl]amino]-2-oxoethyl]-2-[(4-methylphenyl)thio]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C47 H66 N4 O12 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



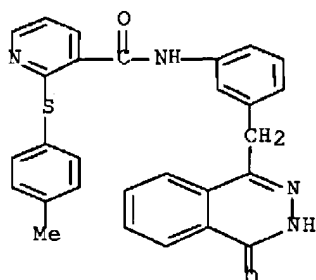
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1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:63420

L31 ANSWER 8 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 420847-48-9 REGISTRY  
CN 3-Pyridinecarboxamide, N-[3-[(3,4-dihydro-4-oxo-1-phthalazinyl)methyl]phenyl]-2-[(4-methylphenyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C28 H22 N4 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

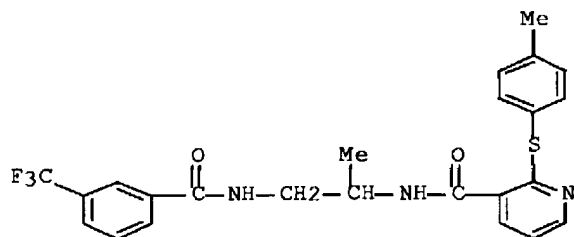


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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:355242

L31 ANSWER 9 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 346669-15-6 REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-methylphenyl)thio]-N-[1-methyl-2-[[3-(trifluoromethyl)benzoyl]amino]ethyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C24 H22 F3 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



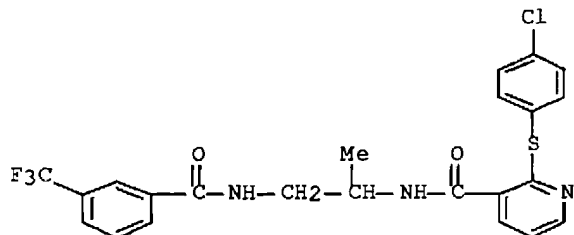
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76694

L31 ANSWER 10 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 346669-13-4 REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[1-methyl-2-[[3-(trifluoromethyl)benzoyl]amino]ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD  
MF C23 H19 Cl F3 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76694

L31 ANSWER 11 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 333990-73-1 REGISTRY

CN 4-Piperidinecarboxamide, N-(3,4-dichlorophenyl)-N-[3-[4-[(4-fluorophenyl)methyl]-1-piperidinyl]propyl]-1-[[2-[(4-methylphenyl)thio]-3-pyridinyl]carbonyl]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

OTHER NAMES:

CN N-(3,4-Dichlorophenyl)-N-[3-[4-(4-fluorobenzyl)-1-piperidinyl]propyl]-1-[2-(4-methylphenylthio)-3-pyridylcarbonyl]-4-piperidinecarboxamide trifluoroacetate (1:3)

MF C40 H43 Cl2 F N4 O2 S . 3 C2 H F3 O2

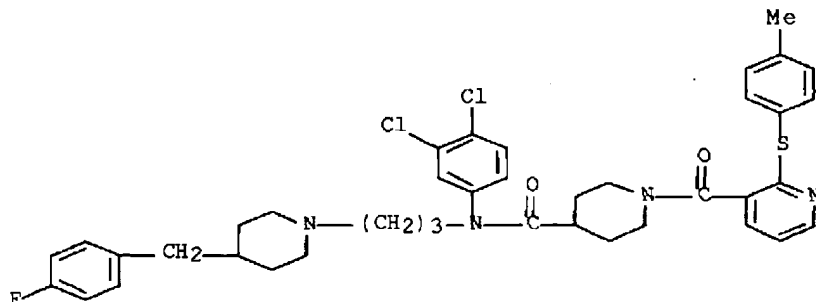
SR CA

LC STN Files: CA, CAPLUS, USPATFULL

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CRN 333990-72-0

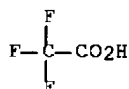
CMF C40 H43 Cl2 F N4 O2 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:295739

L31 ANSWER 12 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 325162-30-9 REGISTRY

CN Benzoic acid, 3-[[[3-[(4-chlorophenyl)methyl]-4-pyridinyl]methylene]amino]-2-methoxy- (9CI) (CA INDEX NAME)

OTHER NAMES:

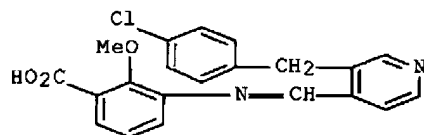
CN 3-[[[3-(4-Chlorobenzyl)-4-pyridyl]methylene]amino]salicylic acid methyl ester

FS 3D CONCORD

MF C21 H17 Cl N2 O3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:163045

L31 ANSWER 13 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 325162-28-5 REGISTRY

CN Benzoic acid, 3-[[[3-[(4-chlorophenyl)methyl]-4-pyridinyl]methyl]amino]-2-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

OTHER NAMES:

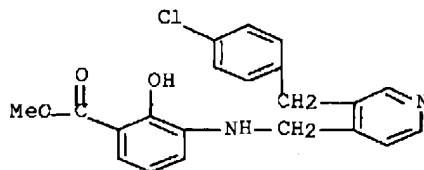
CN 3-[[[3-(4-Chlorobenzyl)-4-pyridyl]methyl]amino]salicylic acid methyl ester

FS 3D CONCORD

MF C21 H19 Cl N2 O3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:163045

L31 ANSWER 14 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 325162-26-3 REGISTRY

CN 2H-1,4-Benzoxazine-8-carboxylic acid, 4-[[3-[(4-chlorophenyl)methyl]-4-pyridinyl]methyl]-3,4-dihydro-, methyl ester (9CI) (CA INDEX NAME)

OTHER NAMES:

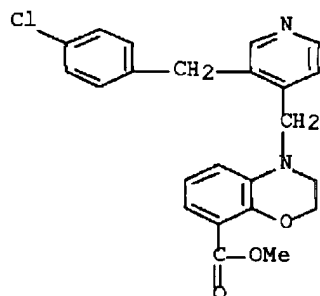
CN 4-[[3-(4-Chlorobenzyl)-4-pyridyl]methyl]-3,4-dihydro-2H-benzo[b][1,4]oxazine-8-carboxylic acid methyl ester

FS 3D CONCORD

MF C23 H21 Cl N2 O3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:163045

L31 ANSWER 15 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 325162-23-0 REGISTRY

CN 2H-1,4-Benzoxazine-8-carboxylic acid, 4-[[3-[(4-chlorophenyl)methyl]-4-pyridinyl]methyl]-3,4-dihydro-, sodium salt (9CI) (CA INDEX NAME)

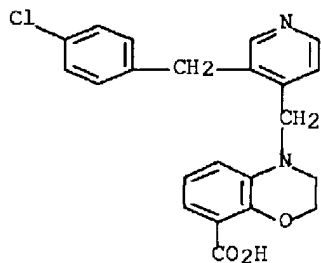
OTHER NAMES:

CN 4-[[3-(4-Chlorobenzyl)-4-pyridyl]methyl]-3,4-dihydro-2H-benzo[b][1,4]oxazine-8-carboxylic acid sodium salt

MF C22 H19 Cl N2 O3 . Na

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER



● Na

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:163045

L31 ANSWER 16 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 325162-21-8 REGISTRY

CN L-Tyrosine, N-[[4-[[3-[(4-chlorophenyl)methyl]-4-pyridinyl]methyl]-3,4-dihydro-2H-1,4-benzoxazin-8-yl]carbonyl]-O-methyl-, methyl ester (9CI)  
(CA INDEX NAME)

OTHER NAMES:

CN N-[1(S)-Methoxycarbonyl-2-(4-methoxyphenyl)ethyl]-4-[[3-(4-chlorobenzyl)-4-pyridyl]methyl]-3,4-dihydro-2H-benzo[b][1,4]oxazine-8-carboxamide

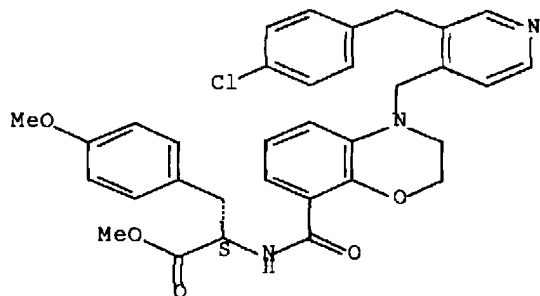
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MF C33 H32 Cl N3 O5

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:163045

L31 ANSWER 17 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 325162-05-8 REGISTRY

CN 2H-1,4-Benzoxazine-8-carboxamide, N-[(1S)-2-amino-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-4-[[3-[(4-chlorophenyl)methyl]-4-pyridinyl]methyl]-3,4-dihydro-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

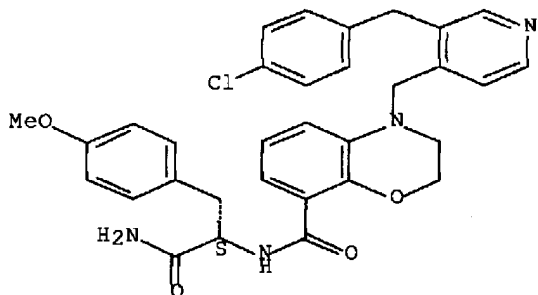
OTHER NAMES:

CN N-[1(S)-Carbamoyl-2-(4-methoxyphenyl)ethyl]-4-[[3-(4-chlorobenzyl)-4-pyridyl]methyl]-3,4-dihydro-2H-1,4-benzoxazine-8-carboxamide oxalate  
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MF C32 H31 Cl N4 O4 . C2 H2 O4  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

CM 1

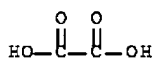
CRN 325160-94-9  
CMF C32 H31 Cl N4 O4

Absolute stereochemistry.



CM 2

CRN 144-62-7  
CMF C2 H2 O4



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:163045

L31 ANSWER 18 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

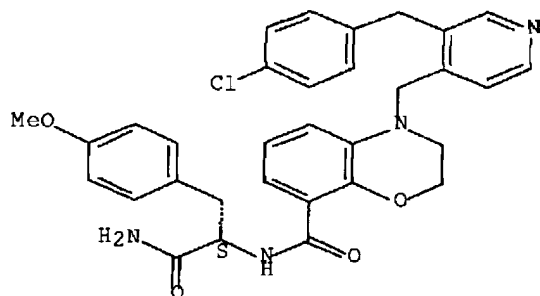
RN 325160-94-9 REGISTRY

CN 2H-1,4-Benzoxazine-8-carboxamide, N-[(1S)-2-amino-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-4-[[3-[(4-chlorophenyl)methyl]-4-pyridinyl]methyl]-3,4-dihydro- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN N-[1-(S)-Carbamoyl-2-(4-methoxyphenyl)ethyl]-4-[[3-(4-chlorobenzyl)-4-pyridyl]methyl]-3,4-dihydro-2H-benzo[b][1,4]oxazine-8-carboxamide  
FS STEREOSEARCH  
MF C32 H31 Cl N4 O4  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

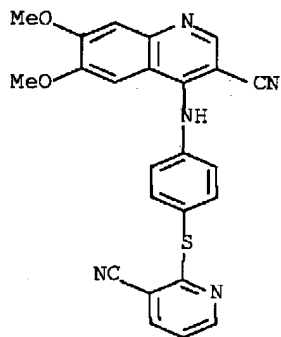


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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:163045

L31 ANSWER 19 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 306999-01-9 REGISTRY  
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MF C24 H17 N5 O2 S  
SR CA  
LC STN Files: CA, CAPLUS



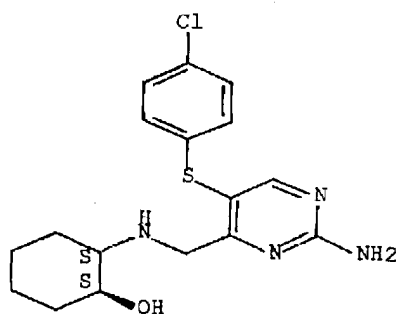
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1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 133:362712

L31 ANSWER 20 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 300855-81-6 REGISTRY  
CN Cyclohexanol, 2-[[[2-amino-5-[(4-chlorophenyl)thio]-4-pyrimidinyl]methyl]amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C17 H21 Cl N4 O S  
SR CA  
LC STN Files: CA, CAPLUS

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

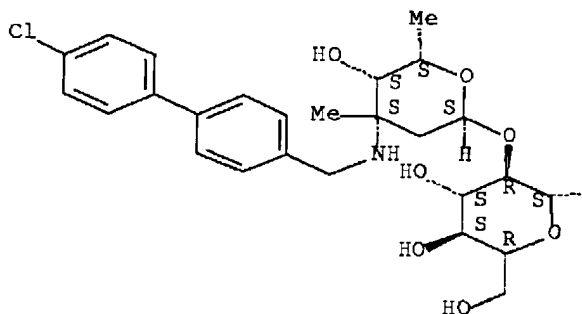
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 133:296442

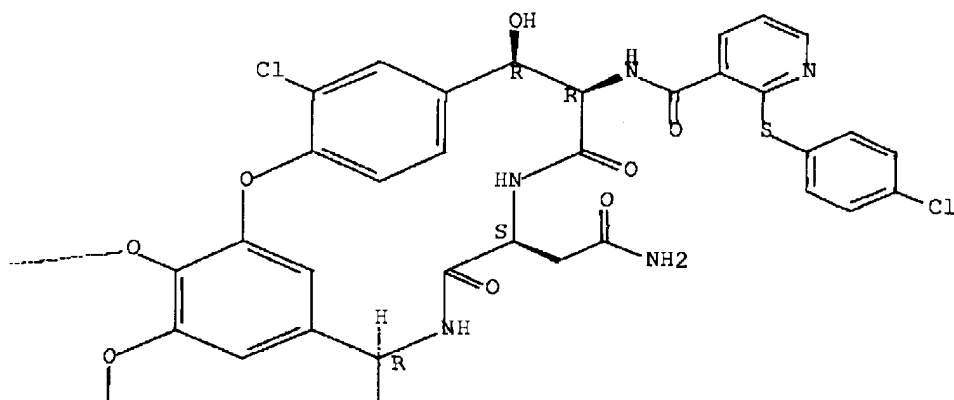
L31 ANSWER 21 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 300581-67-3, REGISTRY  
CN Vancomycin, N3'''-[(4'-chloro[1,1'-biphenyl]-4-yl)methyl]-49-[[2-[(4-chlorophenyl)thio]-3-pyridinyl]carbonyl]-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C84 H77 Cl4 N9 O24 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

PAGE 1-A



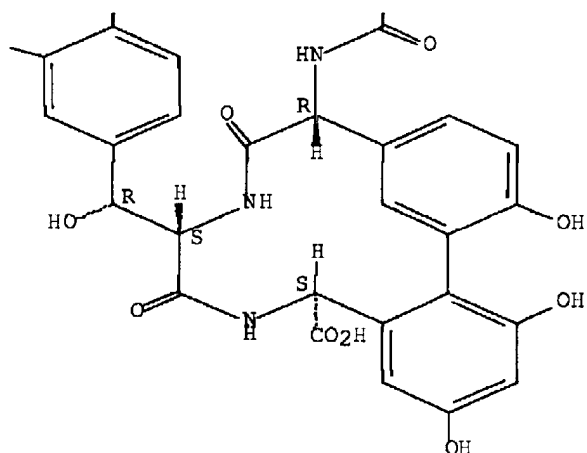
PAGE 1-B



PAGE 2-A

Cl

PAGE 2-B



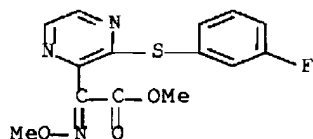
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 133:296658

L31 ANSWER 22 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 259673-23-9 REGISTRY  
CN Pyrazineacetic acid, 3-[(3-fluorophenyl)thio]-.alpha.-(methoxyimino)-, methyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C14 H12 F N3 O3 S  
SR CA

LC STN Files: CA, CAPLUS

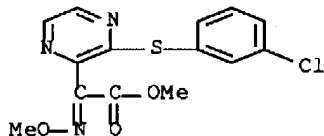


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:180599

L31 ANSWER 23 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 259673-20-6 REGISTRY  
CN Pyrazineacetic acid, 3-[(3-chlorophenyl)thio]-.alpha.-(methoxyimino)-,  
methyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C14 H12 Cl N3 O3 S  
SR CA  
LC STN Files: CA, CAPLUS

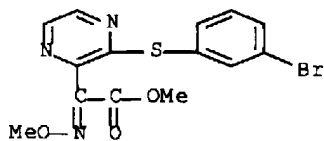


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:180599

L31 ANSWER 24 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 259673-17-1 REGISTRY  
CN Pyrazineacetic acid, 3-[(3-bromophenyl)thio]-.alpha.-(methoxyimino)-,  
methyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C14 H12 Br N3 O3 S  
SR CA  
LC STN Files: CA, CAPLUS

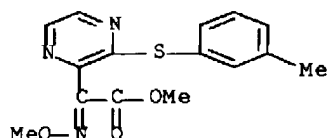


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:180599

L31 ANSWER 25 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **259673-08-0** REGISTRY  
CN Pyrazineacetic acid, .alpha.-(methoxyimino)-3-[(3-methylphenyl)thio]-,  
methyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C15 H15 N3 O3 S  
SR CA  
LC STN Files: CA, CAPLUS

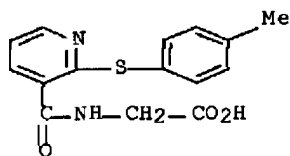


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:180599

L31 ANSWER 26 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **245322-47-8** REGISTRY  
CN Glycine, N-[[2-[(4-methylphenyl)thio]-3-pyridinyl]carbonyl]- (9CI) (CA  
INDEX NAME)  
FS 3D CONCORD  
MF C15 H14 N2 O3 S  
SR CAS Client Services  
LC STN Files: CA, CAPLUS, CHEMCATS, USPATFULL



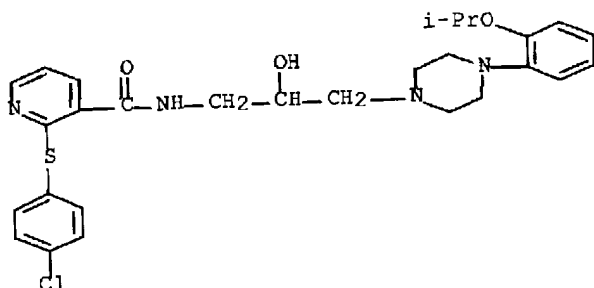
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:63420

L31 ANSWER 27 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **240418-34-2** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[2-hydroxy-3-[4-[2-(1-  
methylethoxy)phenyl]-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD

MF C28 H33 Cl N4 O3 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

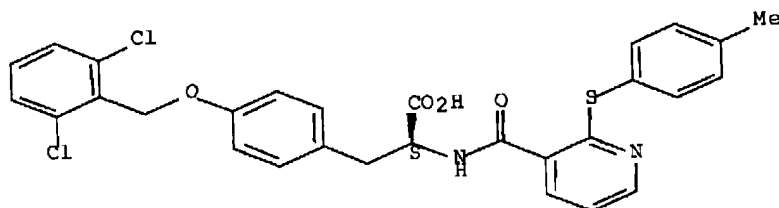
2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:424

REFERENCE 2: 131:184970

L31 ANSWER 28 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 232617-65-1 REGISTRY  
CN L-Tyrosine, O-[(2,6-dichlorophenyl)methyl]-N-[[2-[(4-methylphenyl)thio]-3-pyridinyl]carbonyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H24 Cl2 N2 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



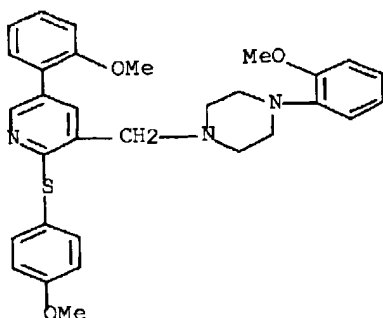
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:116520

L31 ANSWER 29 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 228095-95-2 REGISTRY  
CN Piperazine, 1-(2-methoxyphenyl)-4-[[5-(2-methoxyphenyl)-2-[(4-methoxyphenyl)thio]-3-pyridinyl]methyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C31 H33 N3 O3 S  
SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

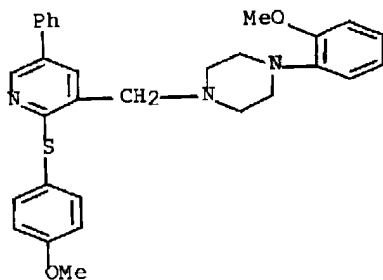
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:58848

L31 ANSWER 30 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 228095-92-9 REGISTRY  
CN Piperazine, 1-(2-methoxyphenyl)-4-[[2-[(4-methoxyphenyl)thio]-5-phenyl-3-pyridinyl]methyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)  
MF C30 H31 N3 O2 S . C2 H2 O4  
SR CA  
LC STN Files: CA, CAPLUS

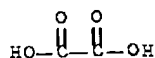
CM 1

CRN 228095-91-8  
CMF C30 H31 N3 O2 S



CM 2

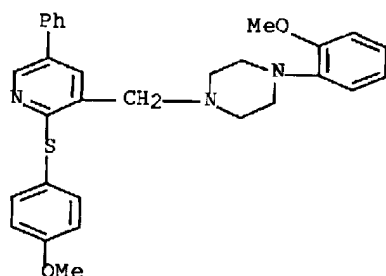
CRN 144-62-7  
CMF C2 H2 O4



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:58848

L31 ANSWER 31 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 228095-91-8 REGISTRY  
CN Piperazine, 1-(2-methoxyphenyl)-4-[[2-[(4-methoxyphenyl)thio]-5-phenyl-3-pyridinyl]methyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C30 H31 N3 O2 S  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS

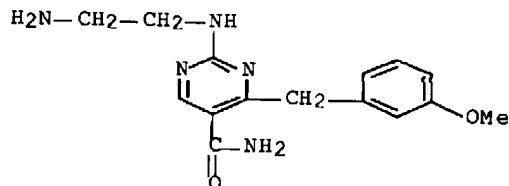


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:58848

L31 ANSWER 32 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 227449-85-6 REGISTRY  
CN 5-Pyrimidinecarboxamide, 2-[(2-aminoethyl)amino]-4-[(3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C15 H19 N5 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

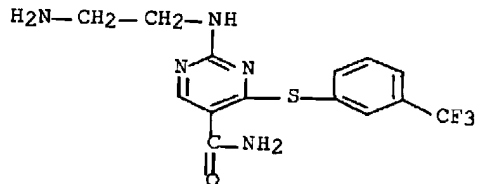


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:44844

L31 ANSWER 33 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **227449-77-6** REGISTRY  
CN 5-Pyrimidinecarboxamide, 2-[(2-aminoethyl)amino]-4-[[3-(trifluoromethyl)phenyl]thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C14 H14 F3 N5 O S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

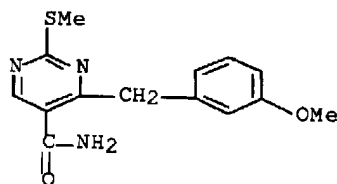


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:44844

L31 ANSWER 34 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **227449-65-2** REGISTRY  
CN 5-Pyrimidinecarboxamide, 4-[(3-methoxyphenyl)methyl]-2-(methylthio)- (9CI)  
(CA INDEX NAME)  
FS 3D CONCORD  
MF C14 H15 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL



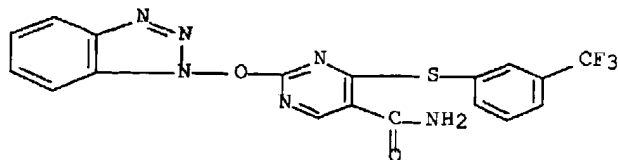
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:44844

L31 ANSWER 35 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **227449-54-9** REGISTRY  
CN 5-Pyrimidinecarboxamide, 2-(1H-benzotriazol-1-yloxy)-4-[[3-(trifluoromethyl)phenyl]thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C18 H11 F3 N6 O2 S

SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

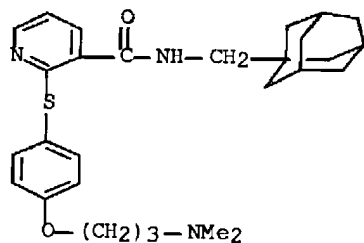


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:44844

L31 ANSWER 36 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **227327-82-4** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[[4-[3-(dimethylamino)propoxy]phenyl]thio]-N-(tricyclo[3.3.1.1.3,7]dec-1-ylmethyl)-, dihydrochloride (9CI) (CA INDEX NAME)  
MF C28 H37 N3 O2 S . 2 Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

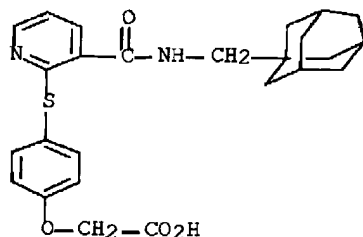


●2 HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:58652

L31 ANSWER 37 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **227327-80-2** REGISTRY  
CN Acetic acid, [4-[[3-[[[tricyclo[3.3.1.1.3,7]dec-1-ylmethyl]amino]carbonyl]-2-pyridinyl]thio]phenoxy]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C25 H28 N2 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

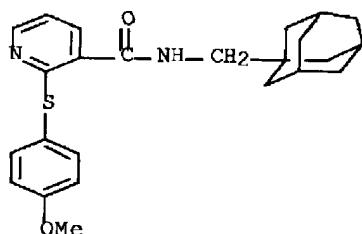


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:58652

L31 ANSWER 38 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **227327-73-3** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-methoxyphenyl)thio]-N-  
(tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-ylmethyl)- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C24 H28 N2 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

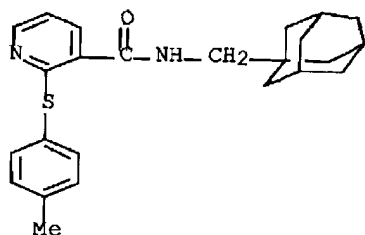


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:58652

L31 ANSWER 39 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **227327-50-6** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-methylphenyl)thio]-N-(tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-ylmethyl)- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C24 H28 N2 O S  
SR CA  
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

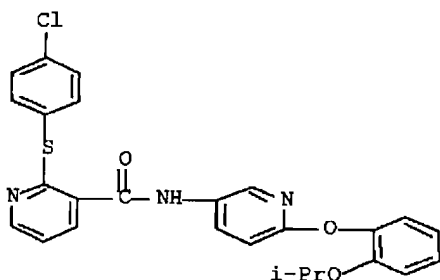


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:58652

L31 ANSWER 40 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224822-03-1** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[6-[2-(1-methylethoxy)phenoxy]-3-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C26 H22 Cl N3 O3 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

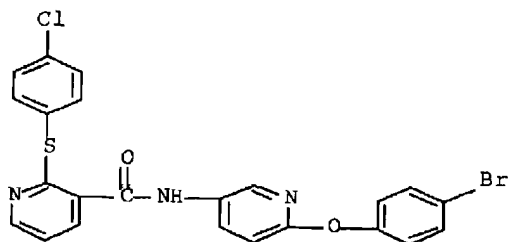


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 41 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224814-98-6** REGISTRY  
CN 3-Pyridinecarboxamide, N-[6-(4-bromophenoxy)-3-pyridinyl]-2-[(4-chlorophenyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H15 Br Cl N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

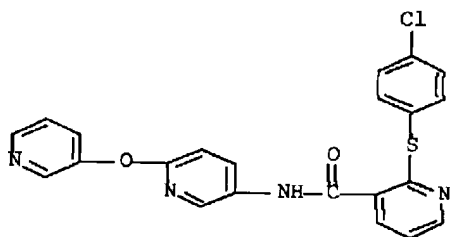


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 42 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224813-98-3** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[6-(3-pyridinyloxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C22 H15 Cl N4 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

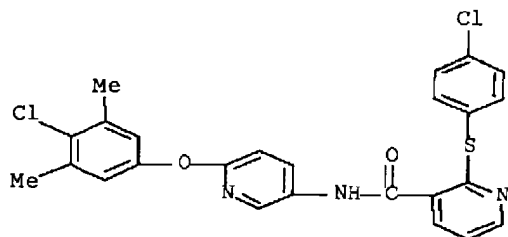


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 43 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224812-92-4** REGISTRY  
CN 3-Pyridinecarboxamide, N-[6-(4-chloro-3,5-dimethylphenoxy)-3-pyridinyl]-2-[(4-chlorophenyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C25 H19 Cl2 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

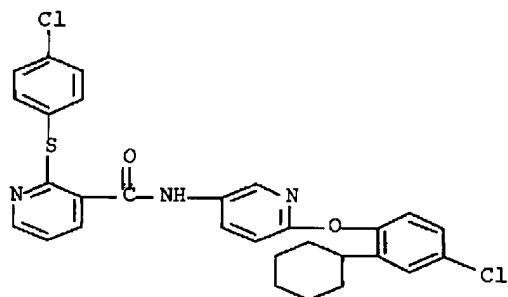


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 44 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224811-52-3** REGISTRY  
CN 3-Pyridinecarboxamide, N-[6-(4-chloro-2-cyclohexylphenoxy)-3-pyridinyl]-2-  
[(4-chlorophenyl)thio]- (9CI) (CA INDEX NAME)  
MF C29 H25 Cl2 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

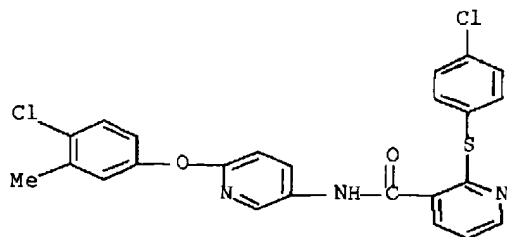


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 45 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224810-57-5** REGISTRY  
CN 3-Pyridinecarboxamide, N-[6-(4-chloro-3-methylphenoxy)-3-pyridinyl]-2-[(4-  
chlorophenyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C24 H17 Cl2 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

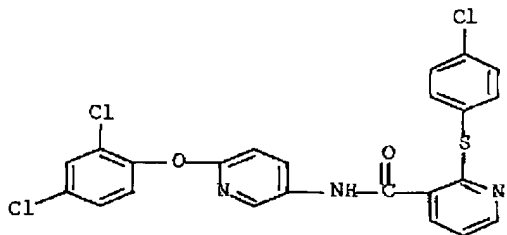


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 46 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224809-64-7** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[6-(2,4-dichlorophenoxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H14 Cl3 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

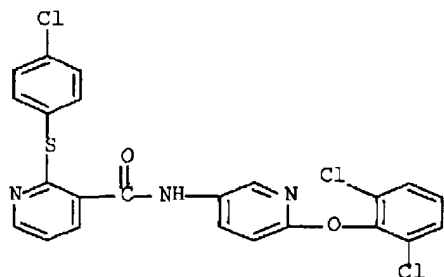


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 47 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224808-46-2** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[6-(2,6-dichlorophenoxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H14 Cl3 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

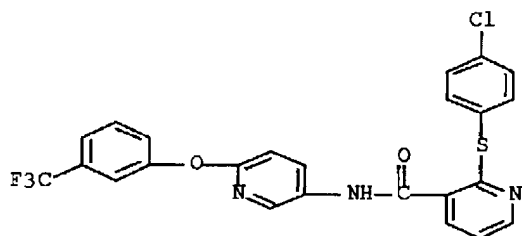


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 48 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224807-56-1** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[6-[3-(trifluoromethyl)phenoxy]-3-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C24 H15 Cl F3 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

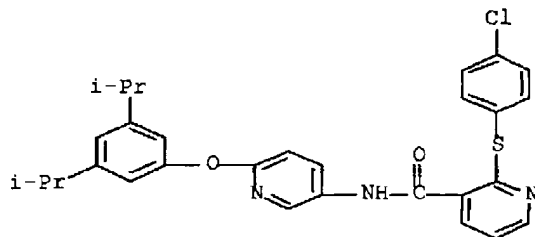


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 49 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224806-63-7** REGISTRY  
CN 3-Pyridinecarboxamide, N-[6-[3,5-bis(1-methylethyl)phenoxy]-3-pyridinyl]-2-[(4-chlorophenyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C29 H28 Cl N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

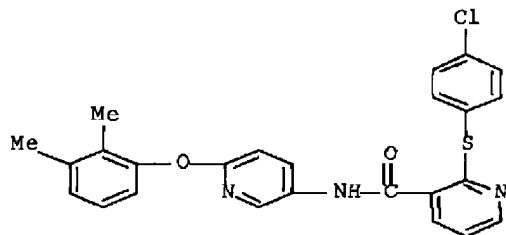


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 50 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224805-72-5** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[6-(2,3-dimethylphenoxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C25 H20 Cl N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

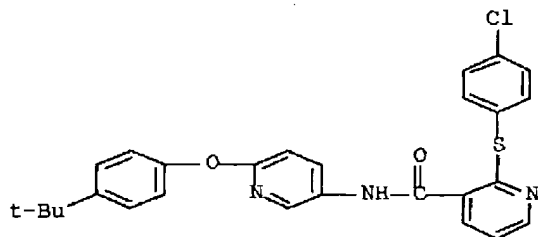


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 51 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224804-80-2** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[6-[4-(1,1-dimethylethyl)phenoxy]-3-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C27 H24 Cl N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

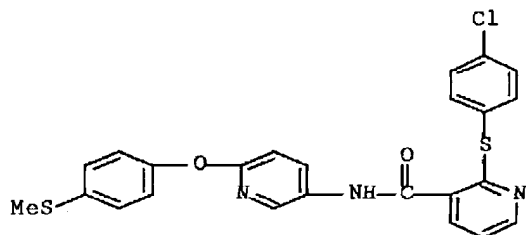


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 52 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224803-75-2** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[6-[4-(methylthio)phenoxy]-3-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C24 H18 Cl N3 O2 S2  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

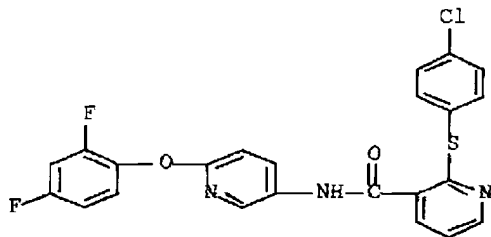


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 53 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224802-65-7** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[6-(2,4-difluorophenoxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H14 Cl F2 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

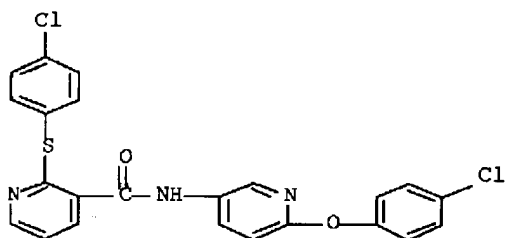


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 54 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 224801-77-8 REGISTRY  
CN 3-Pyridinecarboxamide, N-[6-(4-chlorophenoxy)-3-pyridinyl]-2-[(4-chlorophenyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H15 Cl2 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

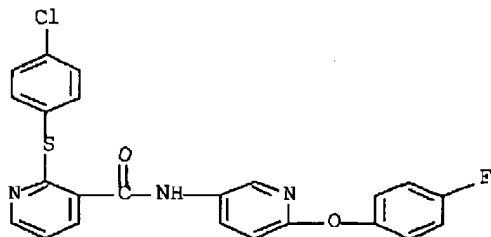


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 55 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 224800-84-4 REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[6-(4-fluorophenoxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H15 Cl F N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

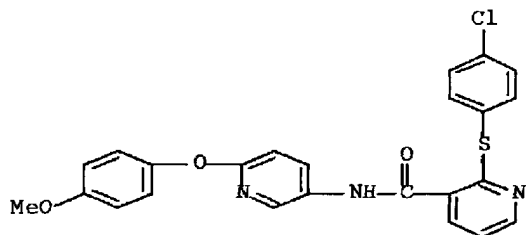


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 56 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224799-37-5** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[6-(4-methoxyphenoxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C24 H18 Cl N3 O3 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

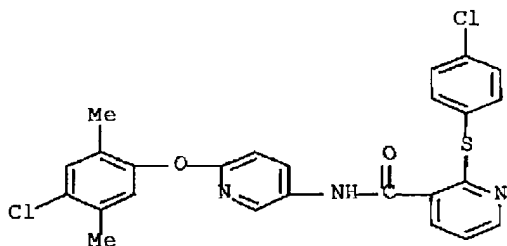


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 57 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **224798-42-9** REGISTRY  
CN 3-Pyridinecarboxamide, N-[6-(4-chloro-2,5-dimethylphenoxy)-3-pyridinyl]-2-[(4-chlorophenyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C25 H19 Cl2 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

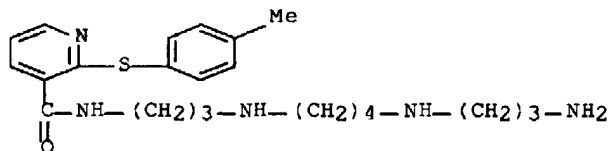


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:352186

L31 ANSWER 58 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 220221-36-3 REGISTRY  
CN 3-Pyridinecarboxamide, N-[3-[[4-[(3-aminopropyl)amino]butyl]amino]propyl]-  
2-[(4-methylphenyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H35 N5 O S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)  
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

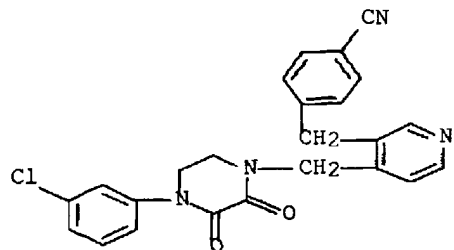
REFERENCE 1: 139:358745

REFERENCE 2: 136:15226

REFERENCE 3: 134:237682

REFERENCE 4: 130:153469

L31 ANSWER 59 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 219919-15-0 REGISTRY  
CN Benzonitrile, 4-[[4-[[4-(3-chlorophenyl)-2,3-dioxo-1-piperazinyl]methyl]-3-  
pyridinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)  
MF C24 H19 Cl N4 O2 . Cl H  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
CRN (197912-97-3)



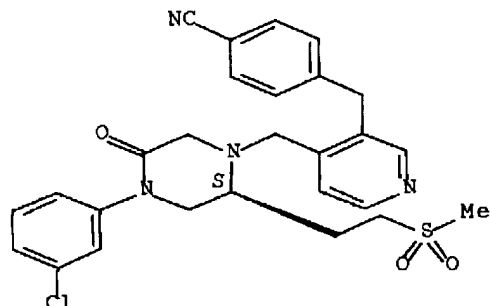
● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:125091

L31 ANSWER 60 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 219552-94-0 REGISTRY  
CN Benzonitrile, 4-[[4-[[[(2S)-4-(3-chlorophenyl)-2-[2-(methylsulfonyl)ethyl]-5-oxo-1-piperazinyl]methyl]-3-pyridinyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C27 H27 Cl N4 O3 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

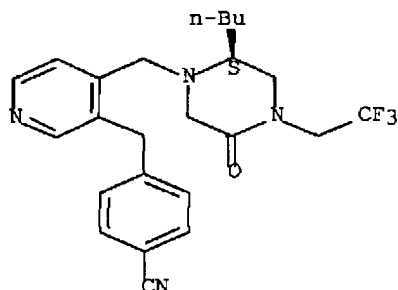
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:95565

L31 ANSWER 61 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 198084-17-2 REGISTRY  
CN Benzonitrile, 4-[[4-[[[(2S)-2-butyl-5-oxo-4-(2,2,2-trifluoroethyl)-1-piperazinyl]methyl]-3-pyridinyl]methyl]-, dihydrochloride (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Benzonitrile, 4-[[4-[[[2-butyl-5-oxo-4-(2,2,2-trifluoroethyl)-1-piperazinyl]methyl]-3-pyridinyl]methyl]-, dihydrochloride, (S)-  
FS STEREOSEARCH  
MF C24 H27 F3 N4 O . 2 Cl H  
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



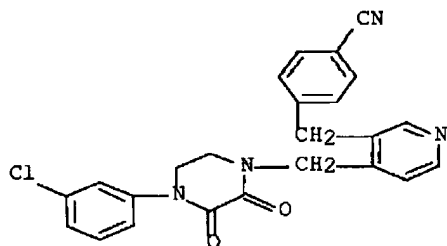
●2 HCl

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:299463

REFERENCE 2: 127:346413

L31 ANSWER 62 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 197912-97-3 REGISTRY  
CN Benzonitrile, 4-[[4-[[4-(3-chlorophenyl)-2,3-dioxo-1-piperazinyl]methyl]-3-pyridinyl]methyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C24 H19 Cl N4 O2  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



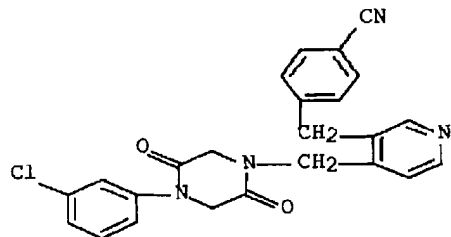
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1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:331505

L31 ANSWER 63 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 197911-53-8 REGISTRY  
CN Benzonitrile, 4-[[4-[[4-(3-chlorophenyl)-2,5-dioxo-1-piperazinyl]methyl]-3-pyridinyl]methyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD  
MF C24 H19 Cl N4 O2  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

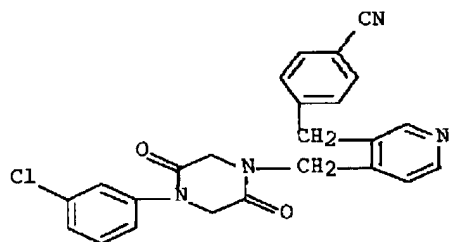


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:331509

L31 ANSWER 64 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 197911-38-9 REGISTRY  
CN Benzonitrile, 4-[[4-[[4-(3-chlorophenyl)-2,5-dioxo-1-piperazinyl]methyl]-3-pyridinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)  
MF C24 H19 Cl N4 O2 . Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
CRN (197911-53-8)

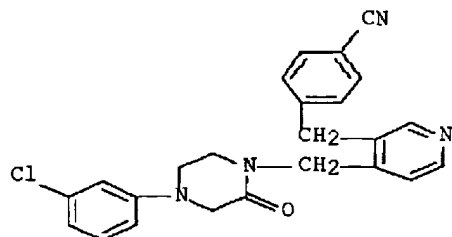


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:331509

L31 ANSWER 65 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 197853-33-1 REGISTRY  
CN Benzonitrile, 4-[[4-[[4-(3-chlorophenyl)-2-oxo-1-piperazinyl]methyl]-3-pyridinyl]methyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C24 H21 Cl N4 O  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL



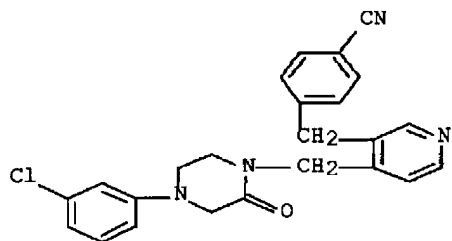
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:237591

REFERENCE 2: 127:331503

L31 ANSWER 66 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 197853-30-8 REGISTRY  
CN Benzonitrile, 4-[[4-[[4-(3-chlorophenyl)-2-oxo-1-piperazinyl]methyl]-3-pyridinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)  
MF C24 H21 Cl N4 O . Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
CRN (197853-33-1)



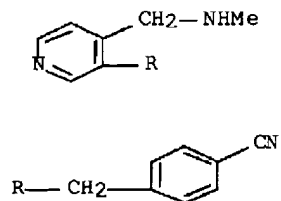
● HCl

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:237591

REFERENCE 2: 127:331503

L31 ANSWER 67 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 197786-45-1 REGISTRY  
CN Benzonitrile, 4-[[4-[(methylamino)methyl]-3-pyridinyl]methyl]- (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN 3-(4-Cyanobenzyl)-4-[(methylamino)methyl]pyridine  
FS 3D CONCORD  
MF C15 H15 N3  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



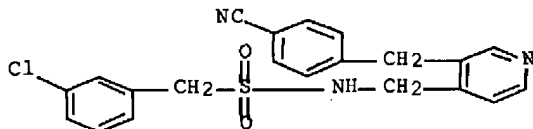
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 129:122662

REFERENCE 2: 127:318953

L31 ANSWER 68 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **197786-35-9** REGISTRY  
CN Benzenemethanesulfonamide, 3-chloro-N-[[3-[(4-cyanophenyl)methyl]-4-pyridinyl]methyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C21 H18 Cl N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



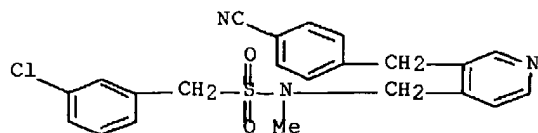
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 129:122662

REFERENCE 2: 127:318953

L31 ANSWER 69 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **197786-28-0** REGISTRY  
CN Benzenemethanesulfonamide, 3-chloro-N-[[3-[(4-cyanophenyl)methyl]-4-pyridinyl]methyl]-N-methyl- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C22 H20 Cl N3 O2 S  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 129:122662

REFERENCE 2: 127:318953

L31 ANSWER 70 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 197786-21-3 REGISTRY

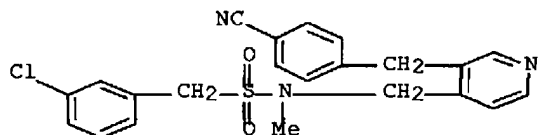
CN Benzenemethanesulfonamide, 3-chloro-N-[[3-[(4-cyanophenyl)methyl]-4-pyridinyl]methyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

MF C22 H20 Cl N3 O2 S . Cl H

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

CRN (197786-28-0)



● HCl

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 129:122662

REFERENCE 2: 127:318953

L31 ANSWER 71 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 182437-80-5 REGISTRY

CN 3-Pyridinecarboxamide, 2-[[4-(4-chlorophenyl)thio]-N-[1-[4-[9-[[2,2,2-trifluoroethyl]amino]carbonyl]-9H-fluoren-9-yl]butyl]-4-piperidinyl]-, dihydrochloride (9CI) (CA INDEX NAME)

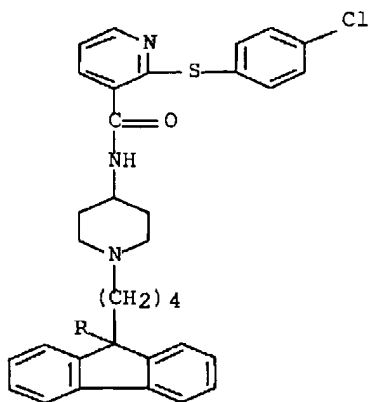
MF C37 H36 Cl F3 N4 O2 S . 2 Cl H

SR CA

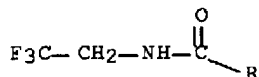
LC STN Files: CA, CAPLUS

CRN (182432-31-1)

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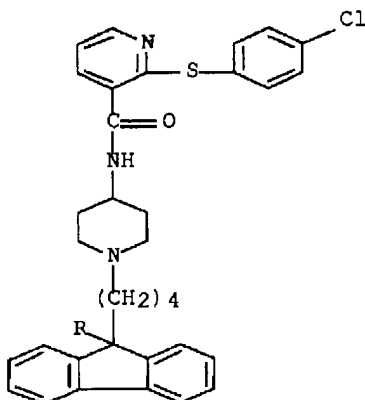
●2 HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

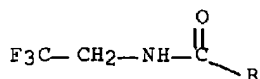
REFERENCE 1: 125:275663

L31 ANSWER 72 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **182436-32-4** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[1-[4-[9-[[2,2,2-trifluoroethyl)amino]carbonyl]-9H-fluoren-9-yl]butyl]-4-piperidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)  
MF C37 H36 Cl F3 N4 O2 S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS  
CRN (182432-31-1)

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PAGE 2-A



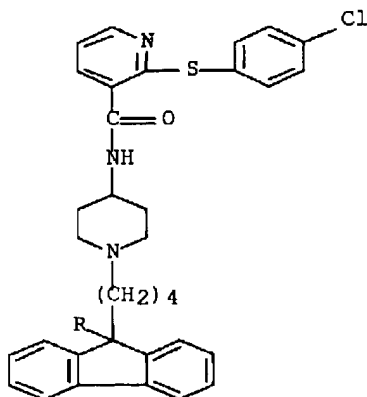
● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

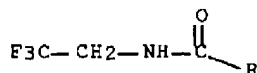
REFERENCE 1: 125:275663

L31 ANSWER 73 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 182432-31-1 REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-[1-[4-[9-[[[2,2,2-trifluoroethyl]amino]carbonyl]-9H-fluoren-9-yl]butyl]-4-piperidinyl]-(9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C37 H36 Cl F3 N4 O2 S  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A



PAGE 2-A



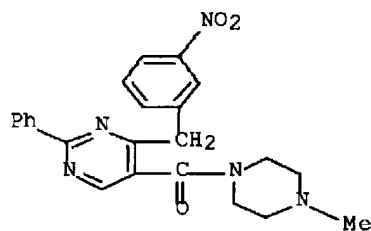
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:154011

REFERENCE 2: 125:275663

L31 ANSWER 74 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 159970-99-7 REGISTRY  
CN Piperazine, 1-methyl-4-[[4-[(3-nitrophenyl)methyl]-2-phenyl-5-pyrimidinyl]carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)  
MF C23 H23 N5 O3 . Cl H  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER  
CRN (116904-78-0)

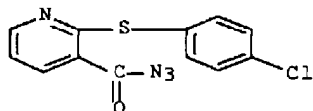


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 122:55996

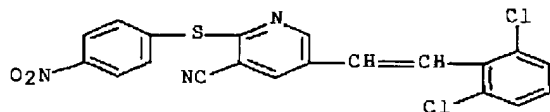
L31 ANSWER 75 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 153143-99-8 REGISTRY  
CN 3-Pyridinecarbonyl azide, 2-[(4-chlorophenyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C12 H7 Cl N4 O S  
SR CA  
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 120:152980

L31 ANSWER 76 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 145769-31-9 REGISTRY  
CN 3-Pyridinecarbonitrile, 5-[2-(2,6-dichlorophenyl)ethenyl]-2-[(4-nitrophenyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C20 H11 Cl2 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

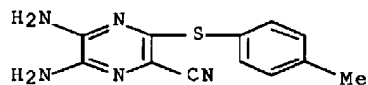


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 118:147572

L31 ANSWER 77 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **143469-45-8** REGISTRY  
CN Pyrazinecarbonitrile, 5,6-diamino-3-[(4-methylphenyl)thio]- (9CI) (CA  
INDEX NAME)  
FS 3D CONCORD  
MF C12 H11 N5 S  
SR CA  
LC STN Files: CA, CAPLUS

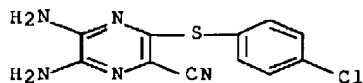


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 117:171474

L31 ANSWER 78 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **143469-44-7** REGISTRY  
CN Pyrazinecarbonitrile, 5,6-diamino-3-[(4-chlorophenyl)thio]- (9CI) (CA  
INDEX NAME)  
FS 3D CONCORD  
MF C11 H8 Cl N5 S  
SR CA  
LC STN Files: CA, CAPLUS



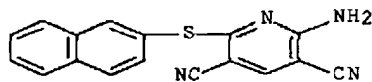
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 117:171474

L31 ANSWER 79 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 141987-66-8 REGISTRY  
CN 3,5-Pyridinedicarbonitrile, 2-amino-6-(2-naphthalenylthio)- (9CI) (CA  
INDEX NAME)  
FS 3D CONCORD  
MF C17 H10 N4 S  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

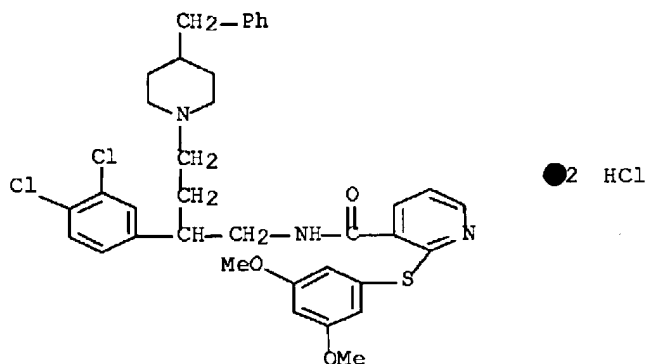


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 117:26413

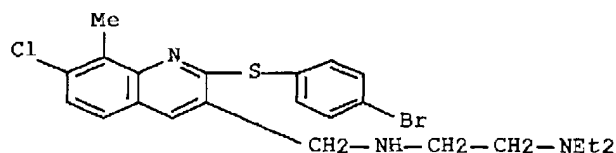
L31 ANSWER 80 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 135956-47-7 REGISTRY  
CN 3-Pyridinecarboxamide, N-[2-(3,4-dichlorophenyl)-4-[4-(phenylmethyl)-1-piperidinyl]butyl]-2-[(3,5-dimethoxyphenyl)thio]-, dihydrochloride (9CI)  
(CA INDEX NAME)  
MF C36 H39 Cl2 N3 O3 S . 2 Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 115:279818

L31 ANSWER 81 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 135629-60-6 REGISTRY  
CN 1,2-Ethanediamine, N'-[[2-[(4-bromophenyl)thio]-7-chloro-8-methyl-3-quinolinyl]methyl]-N,N-diethyl-, monohydrochloride (9CI) (CA INDEX NAME)  
MF C23 H27 Br Cl N3 S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS

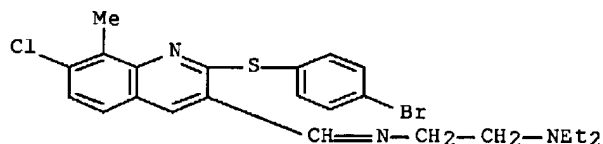


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 115:106008

L31 ANSWER 82 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 135629-48-0 REGISTRY  
CN 1,2-Ethanediamine, N'-[[2-[(4-bromophenyl)thio]-7-chloro-8-methyl-3-quinolinyl]methylene]-N,N-diethyl- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H25 Br Cl N3 S  
SR CA  
LC STN Files: CA, CAPLUS

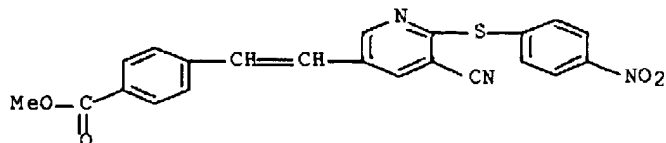


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 115:106008

L31 ANSWER 83 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 135439-27-9 REGISTRY  
CN Benzoic acid, 4-[2-[5-cyano-6-[(4-nitrophenyl)thio]-3-pyridinyl]ethenyl]-, methyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C22 H15 N3 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

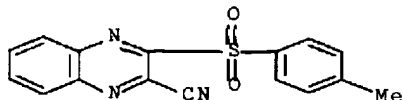


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 115:92864

L31 ANSWER 84 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 128478-59-1 REGISTRY  
CN 2-Quinoxalinecarbonitrile, 3-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C16 H11 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

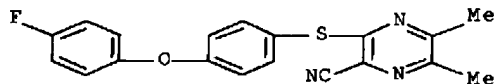


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 113:78340

L31 ANSWER 85 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 128169-38-0 REGISTRY  
CN Pyrazinecarbonitrile, 3-[[4-(4-fluorophenoxy)phenyl]thio]-5,6-dimethyl- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C19 H14 F N3 O S  
SR CA  
LC STN Files: CA, CAPLUS

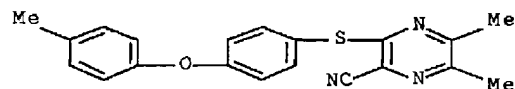


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 113:59240

L31 ANSWER 86 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 128169-37-9 REGISTRY  
CN Pyrazinecarbonitrile, 5,6-dimethyl-3-[[4-(4-methylphenoxy)phenyl]thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C20 H17 N3 O S  
SR CA  
LC STN Files: CA, CAPLUS

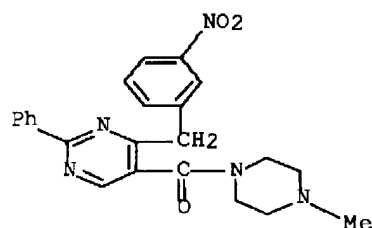


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 113:59240

L31 ANSWER 87 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 116904-78-0 REGISTRY  
CN Piperazine, 1-methyl-4-[[4-[(3-nitrophenyl)methyl]-2-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)  
MF C23 H23 N5 O3  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS

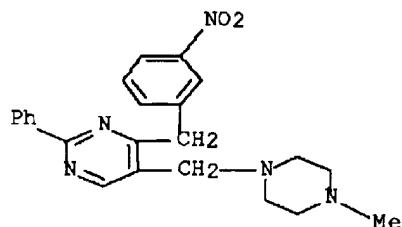


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 109:170451

L31 ANSWER 88 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 116904-66-6 REGISTRY  
CN Pyrimidine, 5-[[4-methyl-1-piperazinyl)methyl]-4-[(3-nitrophenyl)methyl]-2-phenyl- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H25 N5 O2  
SR CA  
LC STN Files: CA, CAPLUS, PROUSDDR, TOXCENTER



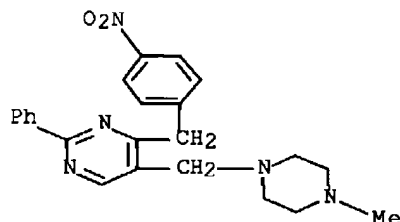
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 122:55996

REFERENCE 2: 109:170451

L31 ANSWER 89 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 116904-65-5 REGISTRY  
CN Pyrimidine, 5-[(4-methyl-1-piperazinyl)methyl]-4-[(4-nitrophenyl)methyl]-2-phenyl- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H25 N5 O2  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



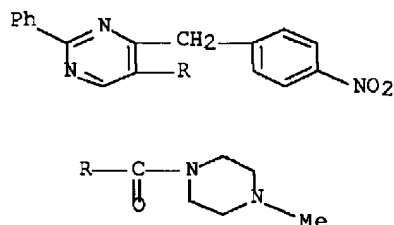
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 122:55996

REFERENCE 2: 109:170451

L31 ANSWER 90 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 116904-35-9 REGISTRY  
CN Piperazine, 1-methyl-4-[[4-[(4-nitrophenyl)methyl]-2-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)  
MF C23 H23 N5 O3  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

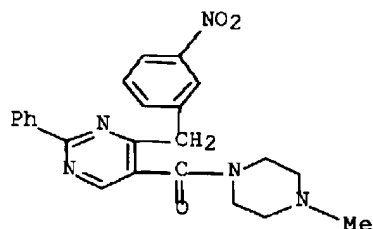
2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 122:55996

REFERENCE 2: 109:170451

L31 ANSWER 91 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 116904-34-8 REGISTRY  
CN Piperazine, 1-methyl-4-[[4-[(3-nitrophenyl)methyl]-2-phenyl-5-pyrimidinyl]carbonyl]-, hydrochloride (9CI) (CA INDEX NAME)  
MF C23 H23 N5 O3 . x Cl H  
SR CA  
LC STN Files: CA, CAPLUS  
CRN (116904-78-0)



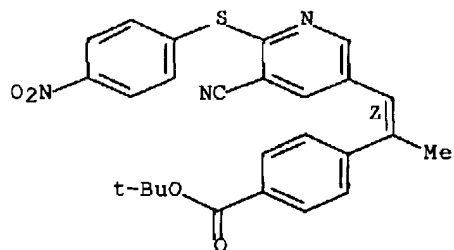
•x HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 109:170451

L31 ANSWER 92 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 105580-43-6 REGISTRY  
CN Benzoic acid, 4-[2-[5-cyano-6-[(4-nitrophenyl)thio]-3-pyridinyl]-1-methylethenyl]-, 1,1-dimethylethyl ester, (Z)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C26 H23 N3 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

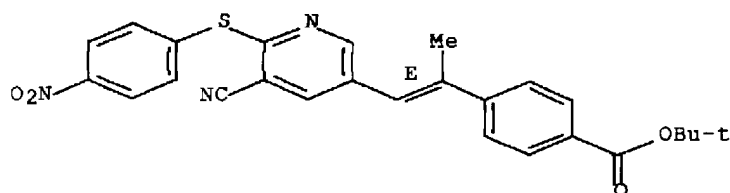
2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 107:176424

REFERENCE 2: 106:33470

L31 ANSWER 93 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 105580-42-5 REGISTRY  
CN Benzoic acid, 4-[2-[5-cyano-6-[(4-nitrophenyl)thio]-3-pyridinyl]-1-methylethenyl]-, 1,1-dimethylethyl ester, (E)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C26 H23 N3 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

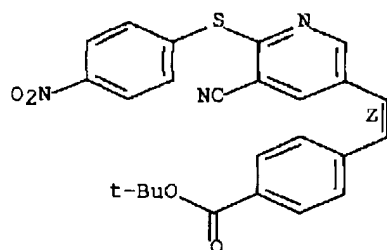
2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 107:176424

REFERENCE 2: 106:33470

L31 ANSWER 94 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 105580-40-3 REGISTRY  
CN Benzoic acid, 4-[2-[5-cyano-6-[(4-nitrophenyl)thio]-3-pyridinyl]ethenyl]-, 1,1-dimethylethyl ester, (Z)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C25 H21 N3 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Double bond geometry as shown.



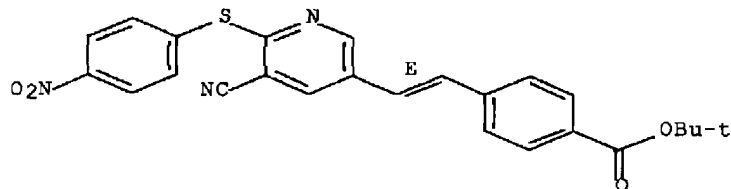
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 106:33470

L31 ANSWER 95 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 105580-39-0 REGISTRY  
CN Benzoic acid, 4-[2-[5-cyano-6-[(4-nitrophenyl)thio]-3-pyridinyl]ethenyl]-, 1,1-dimethylethyl ester, (E)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C25 H21 N3 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Double bond geometry as shown.

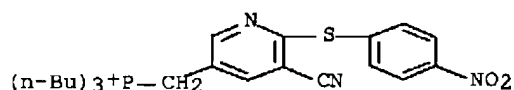


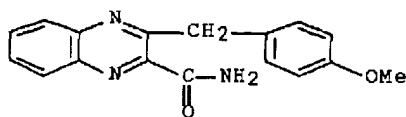
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 106:33470

L31 ANSWER 96 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 105580-38-9 REGISTRY  
CN Phosphonium, tributyl[[5-cyano-6-[(4-nitrophenyl)thio]-3-pyridinyl]methyl]-, bromide (9CI) (CA INDEX NAME)  
MF C25 H35 N3 O2 P S . Br  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL





\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 55:38071

L31 ANSWER 98 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

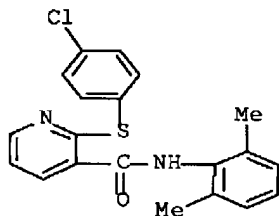
RN 97936-34-0 REGISTRY

CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-(2,6-dimethylphenyl)-  
(9CI) (CA INDEX NAME)

MF C20 H17 Cl N2 O S

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 103:104912

L31 ANSWER 99 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

RN 97936-27-1 REGISTRY

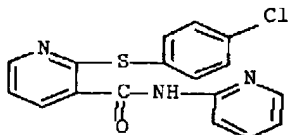
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-2-pyridinyl- (9CI) (CA  
INDEX NAME)

FS 3D CONCORD

MF C17 H12 Cl N3 O S

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

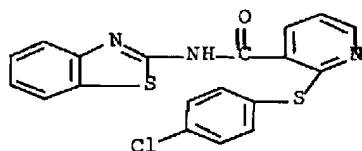


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 103:104912

L31 ANSWER 100 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **97936-26-0** REGISTRY  
CN 3-Pyridinecarboxamide, N-2-benzothiazolyl-2-[(4-chlorophenyl)thio]- (9CI)  
(CA INDEX NAME)  
FS 3D CONCORD  
MF C19 H12 Cl N3 O S2  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

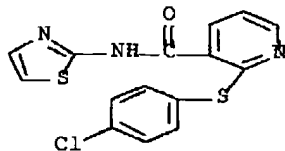


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 103:104912

L31 ANSWER 101 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **97936-25-9** REGISTRY  
CN 3-Pyridinecarboxamide, 2-[(4-chlorophenyl)thio]-N-2-thiazolyl- (9CI) (CA  
INDEX NAME)  
FS 3D CONCORD  
MF C15 H10 Cl N3 O S2  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

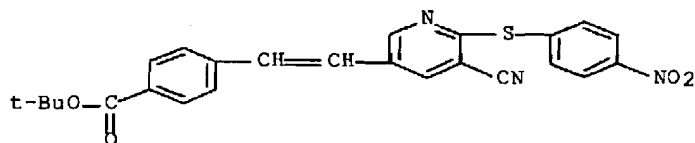


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 103:104912

L31 ANSWER 102 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 95693-78-0 REGISTRY  
CN Benzoic acid, 4-[2-[5-cyano-6-[(4-nitrophenyl)thio]-3-pyridinyl]ethenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C25 H21 N3 O4 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER  
(\*File contains numerically searchable property data)



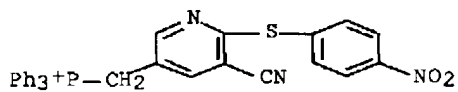
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 107:176424

REFERENCE 2: 103:6676

L31 ANSWER 103 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 95693-77-9 REGISTRY  
CN Phosphonium, [[5-cyano-6-[(4-nitrophenyl)thio]-3-pyridinyl]methyl]triphenyl-, bromide (9CI) (CA INDEX NAME)  
MF C31 H23 N3 O2 P S . Br  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL  
(\*File contains numerically searchable property data)



● Br<sup>-</sup>

4 REFERENCES IN FILE CA (1907 TO DATE)  
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 118:147572

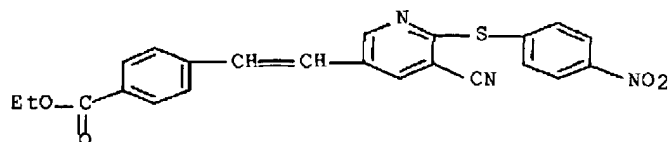
REFERENCE 2: 107:176424

REFERENCE 3: 106:33470

REFERENCE 4: 103:6676

L31 ANSWER 104 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 95674-62-7 REGISTRY  
CN Benzoic acid, 4-[2-[5-cyano-6-[(4-nitrophenyl)thio]-3-pyridinyl]ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H17 N3 O4 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL  
(\*File contains numerically searchable property data)



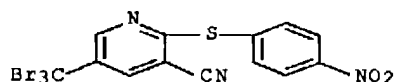
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 106:33470

REFERENCE 2: 103:6676

L31 ANSWER 105 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 88566-70-5 REGISTRY  
CN 3-Pyridinecarbonitrile, 2-[(4-nitrophenyl)thio]-5-(tribromomethyl)- (9CI)  
(CA INDEX NAME)  
FS 3D CONCORD  
MF C13 H6 Br3 N3 O2 S  
LC STN Files: CA, CAPLUS, TOXCENTER

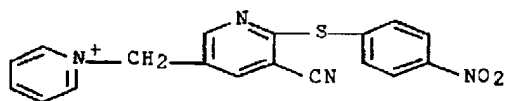


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 100:68665

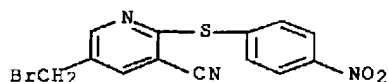
L31 ANSWER 106 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 88553-20-2 REGISTRY  
CN Pyridinium, 1-[[5-cyano-6-[(4-nitrophenyl)thio]-3-pyridinyl]methyl]- (9CI)  
(CA INDEX NAME)  
FS 3D CONCORD  
MF C18 H13 N4 O2 S  
CI COM  
LC STN Files: CA, CAPLUS, TOXCENTER



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 100:68665

L31 ANSWER 107 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 88553-19-9 REGISTRY  
CN 3-Pyridinecarbonitrile, 5-(bromomethyl)-2-[(4-nitrophenyl)thio]- (9CI)  
(CA INDEX NAME)  
FS 3D CONCORD  
MF C13 H8 Br N3 O2 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

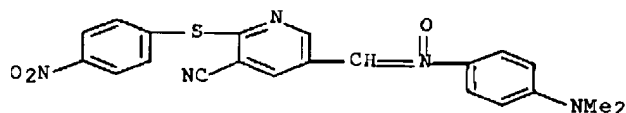
3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 106:33470

REFERENCE 2: 103:6676

REFERENCE 3: 100:68665

L31 ANSWER 108 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 87373-87-3 REGISTRY  
CN 3-Pyridinecarbonitrile, 5-[[[4-(dimethylamino)phenyl]oxidoimino]methyl]-2-  
[(4-nitrophenyl)thio]- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN 3-Pyridinecarbonitrile, 5-[[[4-(dimethylamino)phenyl]imino]methyl]-2-[(4-  
nitrophenyl)thio]-, N-oxide  
FS 3D CONCORD  
MF C21 H17 N5 O3 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

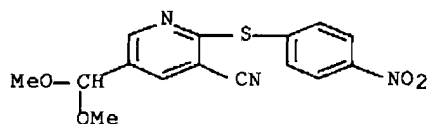
2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 101:55505

REFERENCE 2: 100:103829

L31 ANSWER 109 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 87373-64-6 REGISTRY  
CN 3-Pyridinecarbonitrile, 5-(dimethoxymethyl)-2-[(4-nitrophenyl)thio]- (9CI)  
(CA INDEX NAME)  
FS 3D CONCORD

MF C15 H13 N3 O4 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

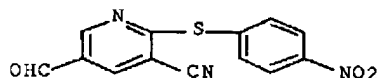
3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 101:55505

REFERENCE 2: 100:103829

REFERENCE 3: 100:68665

L31 ANSWER 110 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 87373-63-5 REGISTRY  
CN 3-Pyridinecarbonitrile, 5-formyl-2-[(4-nitrophenyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C13 H7 N3 O3 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

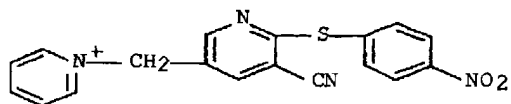
3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 101:55505

REFERENCE 2: 100:103829

REFERENCE 3: 100:68665

L31 ANSWER 111 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 87373-62-4 REGISTRY  
CN Pyridinium, 1-[[5-cyano-6-[(4-nitrophenyl)thio]-3-pyridinyl]methyl]-, bromide (9CI) (CA INDEX NAME)  
MF C18 H13 N4 O2 S . Br  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER  
(\*File contains numerically searchable property data)  
CRN (88553-20-2)



2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 101:55505

REFERENCE 2: 100:103829

L31 ANSWER 112 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

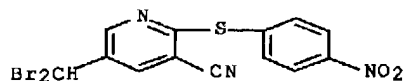
RN 87373-61-3 REGISTRY

CN 3-Pyridinecarbonitrile, 5-(dibromomethyl)-2-[(4-nitrophenyl)thio]- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C13 H7 Br2 N3 O2 S

LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 101:55505

REFERENCE 2: 100:103829

REFERENCE 3: 100:68665

L31 ANSWER 113 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN

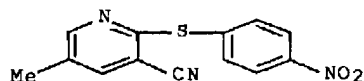
RN 87373-60-2 REGISTRY

CN 3-Pyridinecarbonitrile, 5-methyl-2-[(4-nitrophenyl)thio]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H9 N3 O2 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL  
(\*File contains numerically searchable property data)

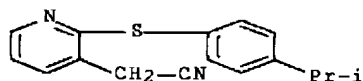


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)  
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 106:33470  
REFERENCE 2: 103:6676  
REFERENCE 3: 101:55505  
REFERENCE 4: 100:103829  
REFERENCE 5: 100:68665

L31 ANSWER 114 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 51723-90-1 REGISTRY  
CN 3-Pyridineacetonitrile, 2-[[4-(1-methylethyl)phenyl]thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C16 H16 N2 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

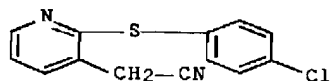


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 85:21451  
REFERENCE 2: 80:82882

L31 ANSWER 115 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 51723-89-8 REGISTRY  
CN 3-Pyridineacetonitrile, 2-[[4-chlorophenyl]thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C13 H9 Cl N2 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CHEMCATS  
(\*File contains numerically searchable property data)



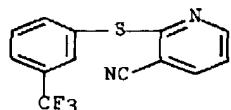
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 85:21451  
REFERENCE 2: 80:82882

L31 ANSWER 116 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 35620-70-3 REGISTRY  
CN 3-Pyridinecarbonitrile, 2-[[3-(trifluoromethyl)phenyl]thio]- (9CI) (CA

INDEX NAME)  
FS 3D CONCORD  
MF C13 H7 F3 N2 S  
LC STN Files: CA, CAPLUS

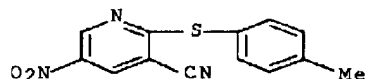


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 76:126788

L31 ANSWER 117 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 31309-29-2 REGISTRY  
CN 3-Pyridinecarbonitrile, 2-[(4-methylphenyl)thio]-5-nitro- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Nicotinonitrile, 5-nitro-2-(p-tolylthio)- (8CI)  
FS 3D CONCORD  
MF C13 H9 N3 O2 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL  
(\*File contains numerically searchable property data)



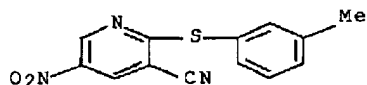
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 77:88314

REFERENCE 2: 74:99891

L31 ANSWER 118 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 31309-28-1 REGISTRY  
CN 3-Pyridinecarbonitrile, 2-[(3-methylphenyl)thio]-5-nitro- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Nicotinonitrile, 5-nitro-2-(m-tolylthio)- (8CI)  
FS 3D CONCORD  
MF C13 H9 N3 O2 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL  
(\*File contains numerically searchable property data)



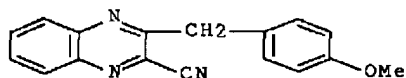
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 77:88314

REFERENCE 2: 74:99891

L31 ANSWER 119 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **23773-91-3** REGISTRY  
CN 2-Quinoxalinecarbonitrile, 3-(p-methoxybenzyl)- (8CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C17 H13 N3 O  
LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

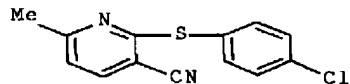


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 71:101819

L31 ANSWER 120 OF 120 REGISTRY COPYRIGHT 2004 ACS on STN  
RN **955-63-5** REGISTRY  
CN Nicotinonitrile, 2-[(p-chlorophenyl)thio]-6-methyl- (7CI, 8CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C13 H9 Cl N2 S  
LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 62:51669